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A GENERAL METHOD FOR CALCULATING
THE SPECIFIC IMPULSE OF
HIGH ENERGY PROPELLANT MIXTURES

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ABSTRACT

~~The method employed by The Dow Chemical Company for calculating specific impulses of propellant mixtures is described. Although the method is general, the capacity of the computer (Burroughs 220) and the availability of thermodynamic data place practical restrictions on what systems can be calculated. The calculations center around the method of White, Johnson, and Dantzig for determining the equilibrium compositions of complex mixtures. By developing and applying matrix equations which describe both the thermodynamic data and the physical equations, the programming effort has been reduced significantly. Required input data to the program are the composition of the reaction mixture, the chamber and exit pressures, and a rough estimate of the chamber temperature. All other pertinent data are retrieved from magnetic tape by the computer program. The program is automatic in that a large number of problems may be solved without manual intervention. In addition to the specific impulse, the program calculates the characteristic velocity, the chamber and exit temperatures, compositions, enthalpies and entropies.~~

the method

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I. INTRODUCTION

The theoretical specific impulse of a propellant system has been used extensively as an indicator to evaluate the maximum performance which could be expected from the system. The calculation of the specific impulse allows rapid and relatively inexpensive screening of the many candidate systems. Earlier work, previously reported^{1,2}, at this Laboratory by R. R. V. Wiederkehr resulted in a general method programmed for a Burroughs 220 Computer.

Recently, the capabilities of the Dow Burroughs 220 were enlarged; therefore, expansion of the computational program was undertaken. The basic mathematical model remained unchanged, but the setup, input, and output sections were extensively revised.

Although the basic method has been discussed in the previously cited reports, for the sake of unity and clarity an exhaustive treatment of the theory and modus operandi of the program will be included in this report.

Specific impulse has been defined as the velocity of the products at the exhaust divided by the gravitational constant. If the change in enthalpy of the chamber products as they are expanded through a nozzle is equated to the kinetic energy of the particles, the specific impulse may be defined as:

$$I_{sp} = c \left[\frac{H_c - H_e}{\mu} \right]^{1/2} \quad (1)$$

where, H_c is the enthalpy of μ grams of products in the rocket chamber,

H_e is the enthalpy of μ grams of products in the nozzle exit, and

c is a constant.

In order to calculate the specific impulse one must merely determine values of H_c and H_e . Assuming no heat losses to the surroundings, a heat balance in which the enthalpy of the reactants is converted to the enthalpy of the products may be written:

$$\sum_{j=1}^p r_j \Delta H_{e_j} = H_c \quad (2)$$

where, r_j is the number of moles of the j th reactant in the reaction mixture,

ΔH_f_j is the heat of formation of the j th reactant at 298°K., and

p is the number of reactants.

To obtain H_e , the equilibrium composition at a chamber temperature must be determined such that equation (2) is satisfied and then an exhaust temperature and composition must be chosen such that there is an entropy balance, $S_c = S_e$, since isentropic flow has been assumed. From this exhaust composition the exit enthalpy, H_e , can be easily calculated as a function of temperature. All the necessary information for the calculation of the specific impulse by equation (1) is then available.

It is recognized that during expansion the reaction products undergo chemical change. The extent of this change cannot be ascertained by theoretical means. It has been assumed, therefore, that complete chemical equilibrium is maintained during the expansion process.

The overall problem may be considered as two separate and identical problems which are merely the determination of a chemical equilibrium composition at a given temperature. The temperatures desired are fixed by the enthalpy balance in the case of the chamber solution and by the entropy balance in the case of the exhaust solution as illustrated in Table I.

Table I

Relation of Temperature with Enthalpy and Entropy Balance

<u>Find T, X such that</u>	<u>Use T, X to Calculate</u>
Chamber: $H(T_c, X_c, P_c) = H_c$	S_c
Exhaust: $S(T_e, X_e, P_e) = S_c$	H_e and I_{sp}

A double trial and error scheme is used to find the desired temperature and composition in each of the two problems. Starting with an assumed temperature, the corresponding equilibrium composition is obtained by a trial and error procedure and then the left side of the equation in Table I is computed using this temperature and composition. If equality is obtained (within practical limits), the assumed temperature is the desired temperature and the composition is the desired composition. If equality is not obtained an improved temperature is assumed.

The magnitude of the improvement is dependent on the magnitude and direction of the inequality. The equilibrium temperature is again calculated and the process repeated until equality is attained.

It is evident that the solution to the problem revolves around a method for determining the compositions and temperatures. This report will consider the following:

- (i) Method for calculating composition (Section II).
- (ii) Method for calculating temperatures (Section III).
- (iii) Method for generating thermodynamic functions (Section IV).
- (iv) Description of the operation, input, output, and capabilities of the computer program.

II. CALCULATION OF THE EQUILIBRIUM COMPOSITION OF A MULTICOMPONENT SYSTEM*

From the first and second laws of thermodynamics it can be shown that a system at constant temperature and pressure achieves equilibrium when the free energy of the system is a minimum. Equilibrium is achieved when the composition is such that the free energy is minimized. This principle is used to calculate the equilibrium compositions of multicomponent systems.

The method used for minimizing the free energy of a system is essentially that of White, Johnson, and Dantzig³ as extended by Thomson⁴ to include condensed species*.

The method performs the following operation: given any composition $Y = (y_1, y_2, y_3 \dots y_n)$ compatible with the mass balance constraints, an improved composition $X = (x_1, x_2, x_3 \dots x_n)$ is calculated which is closer to the equilibrium value. If X is not sufficiently close to the equilibrium value, it becomes the new Y , which can be improved further. The procedure is repeated until convergence is achieved.

*This section is taken almost in its entirety from Report Nr. AR-1S-60, by R. R. V. Wiederkehr (Reference (1)).

A. Composition Convergence Method

The free energy of the system with a composition of X is*:

$$F_r(X) = \sum_{i=1}^{n_g} \left[\left(\frac{F_i}{RT} \right) + \ln P + \ln \frac{x_i}{\bar{x}} \right] x_i + \sum_{i=n_g+1}^{n_g+n_c} \frac{F_i}{RT} x_i \quad (3)$$

$$\text{where, } \bar{x} = \sum_{i=1}^{n_g} x_i \quad (4)$$

The summation in (4) extends over only the gaseous components. The first summation on the right of (3) is the free energy of the gaseous species; the second term is the free energy of the condensed species. The entropy of mixing of the condensed phases is assumed negligible, and the gases are assumed to be ideal.

The behavior of the free energy in the neighborhood of Y may be approximated by a Taylor's expansion, about Y:

$$\begin{aligned} Q(X) = F_r(Y) &+ \sum_{i=1}^{n_g+n_c} \left. \frac{\partial F}{\partial x_i} \right|_{X=Y} (x_i - y_i) \\ &+ 1/2 \sum_{i=1}^{n_g+n_c} \sum_{k=1}^{n_g+n_c} \left. \frac{\partial^2 F}{\partial x_i \partial x_k} \right|_{X=Y} (x_i - y_i)(x_k - y_k) \end{aligned} \quad (5)$$

which reduces to:

$$\begin{aligned} Q(X) = F_r(X) &+ \sum_{i=1}^{n_g} \left[\left(\frac{F_i}{RT} \right) + \ln P + \ln \frac{y_i}{\bar{y}} \right] (x_i - y_i) \\ &+ \sum_{i=n_g+1}^{n_g+n_c} \left(\frac{F_i}{RT} \right) (x_i - y_i) + 1/2 \sum_{i=1}^{n_g} y_i \left[\frac{(x_i - y_i)}{y_i} - (\bar{x} - \bar{y}) \right]^2 \end{aligned} \quad (6)$$

* $F_r(X)$ is actually free energy divided by RT.

It is desired to minimize the quadratic approximation to the free energy $Q(X)$ subject to the element balance restraints given by:

$$\sum_{i=1}^{n_c+n_g} a_{ij}x_i = b_j \quad (7)$$

where a_{ij} are formula numbers indicating the number of atoms of element j in a molecule of species i , and b_j is the total number of atomic weights of element j originally present in the mixture; m is the number of elements in the system.

The constraints and $Q(X)$ may be incorporated into a single equation:

$$G(X) = Q(X) + \sum_{j=1}^m \pi_j \left(\sum_i a_{ij}x_i - b_j \right) \quad (8)$$

where the π_j 's are Lagrange multipliers.

To minimize $G(X)$, $\frac{\partial G}{\partial x_1}$ is set equal to zero. It can be shown via (6) and (8) that for the gaseous components:

$$\frac{\partial G}{\partial x_1} = \left[\left(\frac{F_1}{RT} \right) + \ln P + \ln \frac{y_1}{\bar{y}} \right] + \left[\frac{x_1}{y_1} - \frac{\bar{x}}{\bar{y}} \right] - \sum_{j=1}^m \pi_j a_{1j} = 0 \quad (9)$$

$i=1,2, \dots, n_g$

but for the condensed components:

$$\frac{\partial G}{\partial x_i} = \frac{F_i}{RT} - \sum_{j=1}^m \pi_j a_{ij} = 0 \quad i=n_g+1, n_g+2, \dots, n_g+n_c \quad (10)$$

There are n_g equations of type (9), n_c of type (10), m constraining equations (7), and equation (4). At this point, therefore, there are $n_g + m + 1$ equations and as many unknowns. But by

solving (9) for n_g of the x_1 's and substituting these x_1 's into equations (7) and (4), the number of unknowns is reduced to $n_c + m + 1$. Solving (9) for x_1 yields:

$$x_1 = -y_1 \mathcal{F}_1 + \left(\frac{y_1}{\bar{y}} \right) \bar{x} + \left(\sum_{j=1}^m \pi_j a_{1j} \right) y_1 \quad i=1, 2, \dots, n_g \quad (11)$$

$$\text{where } \mathcal{F}_1 = \left[\left(\frac{F_1}{RT} \right) + \ln P + \ln \frac{y_1}{\bar{y}} \right] \quad (12)$$

Substitution of (11) into (4) and (7) produces:

$$\sum_{j=1}^m \left[\sum_{i=1}^{n_g} a_{ij} y_i \right] \pi_j = \sum_{i=1}^{n_g} y_i \mathcal{F}_i \quad (13)$$

$$\text{and } \sum_{k=1}^m \left[\sum_{i=1}^{n_g} a_{ik} y_i \right] \pi_k + \left[\sum_{i=1}^{n_g} a_{ij} y_i \right] \frac{\bar{x}}{\bar{y}} + \sum_{i=n_g+1}^{n_g+n_c} a_{ij} x_i = b_j + \sum_{i=1}^{n_g} a_{ij} y_i \mathcal{F}_i \quad (14)$$

The problem of minimizing the free energy subject to mass balance constraints reduces to solving equations (14), (10), and (13) simultaneously.

It can be shown that these equations can be rewritten in matrix notation as follows:

$$(A'_g \ Y_{gd} \ A_g) \ \pi + A'_c \ X_c + A'_g \ Y_g \frac{\bar{x}}{\bar{y}} = B + A'_g \ Y_{gD} \mathcal{F}_g \quad (15)$$

$$A_c \pi = \mathcal{F}_c \quad (16)$$

$$Y'_g \ A_g \pi = Y'_g \mathcal{F}_g \quad (17)$$

where the matrices are defined as follows:

$$A_g = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1m} \\ a_{21} & & & \\ \vdots & & & \\ a_{ng,1} & \dots & \dots & a_{ng,m} \end{bmatrix} \quad n_g \times m$$

$$A_c = \begin{bmatrix} a_{ng+1,1} & \dots & a_{ng+1,m} \\ \vdots & & \vdots \\ a_{ng+nc,1} & \dots & a_{ng+nc,m} \end{bmatrix} \quad n_c \times m$$

$$J_g = \begin{bmatrix} \frac{F_1}{RT} \\ \frac{F_2}{RT} \\ \vdots \\ \frac{F_{ng}}{RT} \end{bmatrix} \quad Y_g = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{ng} \end{bmatrix}$$

$$J_c = \begin{bmatrix} \frac{F_{ng+1}}{RT} \\ \frac{F_{ng+2}}{RT} \\ \vdots \\ \frac{F_{ng+nc}}{RT} \end{bmatrix} \quad Y_{GD} = \begin{bmatrix} y_1 & 0 & 0 & \dots & 0 \\ 0 & y_2 & 0 & & \\ 0 & 0 & y_3 & & \\ \vdots & & & \ddots & \\ 0 & \dots & 0 & & y_{ng} \end{bmatrix}$$

$$\pi = \begin{bmatrix} \pi \\ \pi_2 \\ \vdots \\ \pi_m \end{bmatrix} \quad X_g = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{ng} \end{bmatrix}$$

$$B = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix} \quad X_c = \begin{bmatrix} x_{ng+1} \\ \vdots \\ x_{ng+nc} \end{bmatrix}$$

The superscript ¹ designates the transposition of a matrix.

Equations (15), (16) and (17) may be combined to give a single matrix equation:

$$\begin{matrix} m \\ n_c \\ 1 \end{matrix} \left\{ \begin{array}{c|c|c} \overbrace{A'_g \ Y_{gD} \ A_g}^m & \overbrace{A'_c}^{n_c} & \overbrace{A'_g Y_g}^1 \\ \hline & 0 & 0 \\ \hline \overbrace{Y'_g \ A_g}^m & 0 & 0 \end{array} \right\} \begin{bmatrix} \pi \\ X_c \\ \bar{x}/\bar{y} \end{bmatrix} = \begin{bmatrix} B + A'_g Y_{gD} J_g \\ J_c \\ Y'_g J_g \end{bmatrix} \quad (18)$$

This equation represents a system of $m + n_c + 1$ linear equations with as many unknowns. The brackets and symbols indicate the dimensions of the matrices.

The unknowns are: $\pi = (\pi_1, \pi_2, \dots, \pi_m)$,

$X_c = (x_{n_g+1}, x_{n_g+2}, \dots, x_{n_g+n_c})$, and \bar{x}/\bar{y} .

Solving Equation (18) for the unknowns yields:

$$\begin{bmatrix} \pi \\ X_c \\ \bar{x}/\bar{y} \end{bmatrix} = \begin{bmatrix} A'_g \ Y_{gD} \ A_g & A'_c & A'_g Y_g \\ \hline & 0 & 0 \\ \hline Y'_g \ A_g & 0 & 0 \end{bmatrix}^{-1} \begin{bmatrix} B + A'_g Y_{gD} J_g \\ J_c \\ Y'_g J_g \end{bmatrix} \quad (19)$$

The square matrix to be inverted may be calculated from Y and the formula numbers a_{ij} . The vector on the right may be calculated from Y , a_{ij} , and the J_g and J_c vectors. It will be shown in Section IV-A how the J_g and J_c vectors (partial free energy vectors) may be simply calculated. Therefore, given Y , the formula numbers, and the partial free energy vectors, one may calculate: the number of moles of each condensed species at equilibrium, X_c , the Lagrangian multipliers π , and \bar{x}/\bar{y} . The number of moles of each gaseous species at equilibrium may be calculated from Equation (11). In matrix notation Equation (11) is

$$X_g = Y_{gD} \left[\left(\frac{\bar{x}}{\bar{y}} \right) - J_g + A_g \pi \right] \quad (20)$$

where both X_g and $\left[\left(\frac{\bar{x}}{\bar{y}} \right) - J_g + A_g \pi \right]$ are $(n_g \times 1)$ vectors, and Y_{gD} is a $(n_g \times n_g)$ diagonal matrix. In (20) $\left(\frac{\bar{x}}{\bar{y}} \right)$ represents a $(n_g \times 1)$ column matrix whose elements are all $\frac{\bar{x}_i}{\bar{y}}$.

At a given temperature the thermal data and the formula numbers are fixed. Hence, Equations (19) and (20) provide a scheme for obtaining an improved estimate of the equilibrium composition, X, from an original estimate Y. The vector Y may be regarded as an input to our scheme which produces an output X. The resulting X becomes the new Y and the procedure is repeated until X and Y balance.

It is not practical to continue the procedure until an exact balance of X and Y is obtained, since this would take an inordinate amount of time. Therefore, the following criterion is used:

$$\text{If for all } y_i \quad [x_i - y_i]_{\max} < 0.0005 \quad (21)$$

Then X is assumed to be in balance with Y.

B. Convergence Difficulties

Certain difficulties may arise during the process of balancing X and Y, i.e., calculated values of x_i may be negative, the square matrix in equation (9) may fail to invert, or X may continuously oscillate about Y and never quite converge. There follows a discussion of how each of these difficulties may be circumvented.

1. Negative Values of x_i

It sometimes happens that values of x_i calculated by the above method are negative. Physically this has no significance since the number of moles of any species x_i must be zero or positive. To rectify this condition when it occurs, the following procedure is followed:

$$\Delta = X - Y \quad (22)$$

which represents the recommended step needed to improve the compositions. If one or more of the x_i 's are negative the recommended step is too large. Therefore, it is reasonable to merely shorten this recommended step by a factor λ so as to make each of the x_i 's positive. The new values of x_i are given by:

$$X_{\text{new}} = Y + \lambda \Delta \quad (23)$$

for each x_i which is negative let a λ_i be calculated according to the equation.

$$\lambda_i = \frac{-y_i}{\Delta_i} \quad (24)$$

Substitution of this λ_1 into Equation (23) causes x_1 new to be zero. If a λ larger than λ_1 were used, x_1 new would remain negative. Therefore, of all the λ_1 calculated, the smallest must be chosen. This value of λ , viz., λ_s , will cause x_s new to be zero, and all other x_i 's to be positive.

a. Gaseous Species - For gaseous species, zero is an objectionable value to use for x_s since, according to equation (20), this estimate can never be improved but will remain zero. Instead of letting x_s go to zero, the following scheme is used: Arbitrarily values are given to x_s depending on the size of the corresponding y_s , that is,

$$\text{if } y_s > 1 \times 10^{-11}, \quad x_s = 1 \times 10^{-11} \quad (25a)$$

or

$$\text{if } 1 \times 10^{-11} > y_s > 1 \times 10^{-31}, \quad x_s = 1 \times 10^{-31} \quad (25b)$$

or

$$\text{if } y_s < 1 \times 10^{-31}, \quad x_s = 0 \quad (25c)$$

If y_s is small enough, x_s does become zero. Since this would preclude the possibility of any further modification or improvement to this species, when convergence has been attained all zero values are arbitrarily set at a value of 1×10^{-6} and the iteration repeated until X and Y balance again. This device is a radical departure from the previously reported method¹ and has proved to be more efficient. Every time a new temperature is used the device,

$$\text{if } x_i = 0, y_i \text{ new} = 1 \times 10^{-6} \quad (26)$$

is also used.

b. Condensed Species - For condensed species a zero value for x_s is not objectionable. Consequently, using λ_s alone is sufficient.

Another difficulty may arise, however. If x_i for a condensed species is zero (which means y_i for the next iteration is also zero) and the following x_i is negative, an impasse is reached.

Clearly λ_1 calculated from Equation (24) is zero so that $X_{\text{new}} = Y_{\text{old}}$ [see Equation (23)]. A λ of zero prevents X from improving.

III. CALCULATION OF THE CHAMBER AND EXIT TEMPERATURES

Two temperatures, the chamber temperature and the exhaust temperature, must be determined in the course of the solution of the problem. The desired temperature is obtained when the enthalpy of entropy of the system equals the chamber enthalpy or entropy respectively (See Table I). Since the methods used for the two temperatures are similar, only the case of the chamber temperature will be considered.

Starting with an assumed temperature, T , the enthalpy of the system is calculated and compared with the chamber enthalpy. If the calculated enthalpy is low (high), then the next temperature is increased (decreased). This new "improved temperature," T_{n+1} is calculated according to the following linear interpolation or extrapolation formula:

$$T_{n+1} = T_n + \phi_H(H_c - H_n) \quad (27)$$

where H_n is given by Equation (55) and H_c is given by Equation (2). To calculate the second temperature from the assumed first temperature a value for ϕ_H of 0.01 +K./cal. is used. For succeeding temperature ϕ_H is given by:

$$\phi_H = \frac{T_n - T_{n-1}}{H_n - H_{n-1}} \quad (28)$$

Equation (27) is used for extrapolation to new temperature until the chamber temperature has been straddled. Once the chamber temperature has been straddled, Equation (28) is used for interpolation.

Equation (27) has certain shortcomings. When the temperatures T_n and T_{n-1} straddle both the chamber temperature and a phase transition temperature, Equation (27) produces a very poor "improved temperature." This is a result of the very non-linear behavior of H with T in the neighborhood of a phase transition; the enthalpy abruptly changes across the transition (See Figure 1). When this difficulty arises it can be eliminated by the following method which is based on Figure 1.

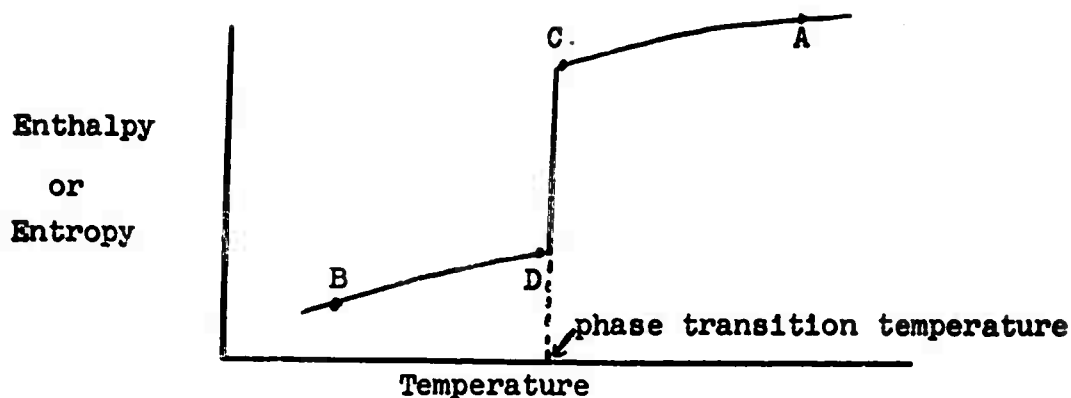


Fig. 1 - Schematic of Non-Linear Behavior of Enthalpy with Temperature

Suppose that the two temperatures which straddle both the chamber temperature and a phase transition temperature yield the points A and B on Figure 1. By calculating the enthalpy of the system at a temperature slightly (0.5°K.) above and below the phase transition temperature, the points C and D are obtained. If the chamber enthalpy is between the enthalpies of points A and C or B and D, Equation (27) is applied using the points A and C or B and D, respectively. However, if the chamber enthalpy lies between the enthalpies of points C and D, then the chamber temperature coincides with the phase transition temperature and the compound undergoing the phase transition must be partly in one phase and partly in the other.

In general, the composition of the system varies upon traversing a phase transition. The phase transition composition (chamber composition) may be calculated on the assumption that the composition varies linearly with the enthalpy across the transition. From the enthalpies and compositions corresponding to C and D and the chamber enthalpy, the chamber composition can be calculated.

To this point the discussion has been concerned with choosing improved temperatures. When an improved temperature T is obtained such that:

$$H(T, X) - H_c < 100 \text{ cal.} \quad (29)$$

then that temperature T is defined as the chamber temperature T_c . In the above equation $H(T, X)$ is given by (55) and H_c is given by (2). The convergence criterion for the exhaust solution is:

$$\text{If } S(T, X, P_e) - S_c < 0.02 \text{ e.u.} \quad (30)$$

then the temperature is the exit temperature. In this equation S_c is evaluated according to (65) using the chamber conditions and $S(T, X, P_e)$ is calculated by (65) at the assumed exit conditions.

IV. THE GENERATION OF THERMODYNAMIC PROPERTIES BY THE USE OF MATRICES

A. The Matrix Representation of the Enthalpy, Entropy, and Free Energy*

To calculate the chamber conditions it is necessary to be able to evaluate the enthalpy as a function of temperature, composition, and pressure. To calculate the exit conditions it is necessary to be able to evaluate the entropy as a function of temperature, composition, and pressure. To calculate the equilibrium composition it is necessary to know the partial free energies as a function of temperature, pressure, and composition. This section shows how these thermodynamic functions can be concisely represented and simply generated by the use of matrices.

1. Single Species System

The enthalpy of a single species (i.e., a compound in a given phase) at a given pressure as a function of temperature can be evaluated if the heat capacity as a function of temperature and the enthalpy at some base temperature, T_b , are known:

$$H(T) = H(T_b) + \int_{T_b}^T C_p(T) dT \quad (31)$$

The molar entropy of a species as a function of temperature at a given pressure can also be evaluated if the heat capacity as a function of temperature and the entropy at some base temperature, T_b , are known:

$$S(T) = S(T_b) + \int_{T_b}^T \frac{C_p(t)}{T} dT \quad (32)$$

The molar free energy of a compound can be evaluated according to the equation:

$$F(T) = H(T) - TS(T) \quad (33)$$

Therefore, given the heat capacity as a function of temperature, and the enthalpy and entropy at some base temperature, T_b , one can evaluate the enthalpy, entropy, and free energy as functions of temperature at a given pressure.

*This section is also taken in its entirety from R. R. V. Wiederkehr, Report No. AR-1s-60.

Maier and Kelly* have successfully described the heat capacity as a function of temperature using the equation:

$$C_p = a + bT + \frac{c}{T^2} \quad (34)$$

where a, b, and c are constants determined from experimental data.

Thompson⁴ has arrived at a significantly improved expression for the heat capacity, viz.,

$$C_p = a + bT + cT^2 + dT^3 + eT^{-2} \quad (35)$$

More generally the heat capacity can be represented by a function which is linear with respect to the parameters, viz.,

$$C_p = \sum_{j=1}^N l_j f_j(T) \quad (36)$$

where the l_j 's are constants* corresponding to the a, b, c's and the $f_j(T)$'s are pure temperature functions. Equations (34) and (35) are specific cases of Equation (36).

If (36) is substituted into (31) and (32) then

$$H(T) = H(T_b) + \sum_{j=1}^N l_j \int_{T_b}^T f_j(T) dT \quad (37)$$

and

$$S(T) = S(T_b) + \sum_{j=1}^N l_j \int_{T_b}^T \frac{f_j(T)}{T} dT \quad (38)$$

If the integrals in (37) and (38) are defined by:

$$I_j(T) = \int f_j(T) dT \quad (39)$$

$$J_j(T) = \int \frac{f_j(T)}{T} dT \quad (40)$$

*At a given pressure the l_j 's are constant.

then substitution of the limits of integration into (39) and (40) leads to

$$H(T) = H(T_b) - \sum_{j=1}^N l_j I_j(T_b) + \sum_{j=1}^N l_j I_j(T) \quad (41)$$

and

$$S(T) = S(T_b) - \sum_{j=1}^N l_j J_j(T_b) + \sum_{j=1}^N l_j J_j(T) \quad (42)$$

Now if the following definitions are introduced

$$\left. \begin{aligned} l_{N+1} &\equiv H(T_b) - \sum_{j=1}^N l_j I_j(T_b) & (a) \\ I_{N+1} &\equiv 1 & (b) \\ J_{N+1} &\equiv 0 & (c) \end{aligned} \right\} \quad (43)$$

$$\left. \begin{aligned} l_{N+2} &\equiv S(T_b) - \sum_{j=1}^N l_j J_j(T_b) & (a) \\ I_{N+2} &\equiv 0 & (b) \\ J_{N+2} &\equiv 1 & (c) \end{aligned} \right\} \quad (44)$$

then (41) becomes

$$H(T) = \sum_{j=1}^{N+2} l_j I_j(T) \quad (45)$$

and (42) becomes

$$S(T) = \sum_{j=1}^{N+2} l_j J_j(T) \quad (46)$$

Substitution of (45) and (46) into (33) yields an expression for the free energy.

$$F(T) = \sum_{j=1}^{N+2} l_j K_j(T) \quad (47)$$

where

$$K_j(T) \equiv I_j(T) - T J_j(T) \quad (48)$$

The equations for H , S , and F apply to a single compound in a single phase, i.e., a single species. The l_j 's may be interpreted as elements of a thermodynamic property vector, \bar{I} , which is independent of temperature. The I_j , J_j , K_j may be interpreted as elements enthalpy, entropy and free energy thermal vectors \bar{I} , \bar{J} , \bar{K} , which depend only on temperature and are independent of the compound. The inner product of \bar{I} with \bar{I} , \bar{J} and \bar{K} yield the enthalpy, entropy and free energy, respectively.

Before the above Equations (45), (46), (47) can be of any practical use, the vectors \bar{I} , \bar{J} , \bar{K} and \bar{I} must be evaluated. All of these vectors depend on the linear form chosen to represent the heat capacity data (Equation 36).

In Appendix I, these vectors are calculated using the linear form proposed by Thomson (Equation 35) and thermodynamic property vectors are tabulated for all of the high temperature combustion products for which data are readily available.

2. Multicomponent Systems:

For the i th species in a multicomponent system in which mixing effects are negligible, the enthalpy, entropy and free energy are:

$$H_i = \sum_{j=1}^{N+2} l_{ij} I_j \quad (49)$$

$$S_i = \sum_{j=1}^{N+2} l_{ij} J_j \quad (50)$$

$$F_i = \sum_{j=1}^{N+2} l_{ij} K_j \quad (51)$$

The total enthalpy of the system is:

$$H = \sum_{i=1}^n x_i H_i \quad (52)$$

where x_i is the number of moles of the i th species present in the system and n is the number of species in the system. Similar expressions hold for the total entropy and total free energy of the system. Substitution of (49) into (52) yields:

$$H = \sum_{i=1}^n x_i \sum_{j=1}^{N+2} l_{ij} I_j \quad (53)$$

or in terms of matrices:

$$H = [x_1, x_2, \dots, x_n] \begin{bmatrix} l_{11} & l_{12} & \dots & l_{1,N+2} \\ l_{21} & & & \\ \vdots & & & \\ l_{n1} & & \dots & l_{n,N+2} \end{bmatrix} \begin{bmatrix} I_1 \\ I_2 \\ \vdots \\ I_{N+2} \end{bmatrix} \quad (54)$$

or, more simply:

$$H = X' L I \quad (55)$$

where X' , L and I are the matrices defined by (54) and (55). Similarly, matrix expressions for the total entropy and total free energy of the system may be written:

$$S = X' L J \quad (56)$$

$$F = X' L K \quad (57)$$

The matrix L is seen to be an array of the thermodynamic property vectors of the species present in the system. Henceforth, the matrix L shall be referred to as the thermodynamic property matrix.

Equations (55), (56) and (57) suffer from the fact that mixing effects have been neglected. Mixing can be accounted for by making the following simplifying assumptions:

1. All gaseous species behave ideally.
2. Condensed species have zero enthalpies and entropies of mixing.

For a mixture of ideal gases, the enthalpy of mixing is zero. The entropy of mixing of the i th species, however, is:

$$\Delta S_1 = - R \rho_1 \quad (58)$$

where

$$\rho_1 = \ln x_1 + \ln \frac{P}{\bar{X}} \quad (59)$$

Consequently, the corrected entropy and free energy per mole of the i th gaseous species are:

$$\bar{S}_1 = S_1 - R \rho_1 \quad (60)$$

$$\bar{F}_1 = F_1 + RT \rho_1 \quad (61)$$

respectively. These corrected values are also partial molar quantities.

Equations (60) and (61) are applicable to condensed species as well as the gaseous species if it is understood that

$$\rho_1 = 0 \quad (62)$$

for all condensed species. Therefore, Equations (49), (60) and (61) may be regarded as being general expressions for the partial molar enthalpy, entropy and free energy of the i th species of a multicomponent system. Substitution of (60) into (50) and (61) into (51), respectively, produces:

$$\bar{S}_1 = \sum_{j=1}^N l_{1j} J_j - R \rho_1 \quad (63)$$

and

$$\bar{F}_1 = \sum_{j=1}^N l_{1j} K_j + RT \rho_1 \quad (64)$$

The results of this section can now be applied to the overall specific impulse calculations.

To determine the chamber and exit temperatures it is necessary to be able to evaluate the enthalpy and entropy as functions of temperature and composition (the pressure is given). Equation (55) provides a very simple means of evaluating the enthalpy.

$$H(T, X) = X' L I \quad (55)$$

If Equation (56) is corrected for mixing according to (63), the following matrix equation for evaluating the entropy is obtained:

$$S(T, P, X) = X' [LJ - RP] \quad (65)$$

In Equation (18), which is used to calculate an improved composition convergence, the vectors \mathcal{J}_g and \mathcal{J}_c are required. Both of these vectors can be generated at once by the use of Equation (64) divided by RT . In matrix notation this equation becomes:

$$\begin{matrix} n_g \{ \overbrace{\begin{bmatrix} \mathcal{J}_g \\ \vdots \\ \mathcal{J}_c \end{bmatrix}}^1 \\ n_c \{ \end{matrix} = \begin{matrix} \overbrace{\begin{bmatrix} L \end{bmatrix}}^{N+2} \end{matrix} \begin{matrix} \overbrace{\begin{bmatrix} K^* \end{bmatrix}}^1 \\ + \begin{matrix} \overbrace{\begin{bmatrix} \mathcal{P}_g \\ \vdots \\ \mathcal{P}_c \end{bmatrix}}^1 \end{matrix} \quad (66)$$

where $K^* = \frac{K}{RT}$

The subscripts g and c refer to the gaseous and condensed species, respectively, and the dimensions of the matrices are designated in the equations by brackets. The vector \mathcal{P}_c is zero.

Equations (55), (65) and (66) are the main results of this section. These equations require that the matrices L , I , J , K , \mathcal{P} and X are given. Elements of the matrix L are independent of temperature, pressure* and composition. For a given problem, therefore, L is invariant. The temperature determines the vectors \mathcal{I} , \mathcal{J} , \mathcal{K} while the pressure and composition determine the vector \mathcal{P} . The vector X , of course, is the composition. Appendix I is concerned with evaluating the vectors \mathcal{I} , I , J , and K .

B. Arrangement of the Product Species and the Construction of the Thermodynamic Property Matrix, L .

The matrix L , which is composed of the \mathcal{I} vectors, depends on how the \mathcal{I} vectors are arranged. Since each \mathcal{I} corresponds to one of the product species, the matrix L depends on how the product species are arranged.

In the method for calculating the equilibrium composition described in Section II, a strong distinction was made between

*The elements of L are actually functions of pressure; but at high temperature the variations of the l_{ij} with pressure are probably small.

gaseous species and condensed species. One type of equation was used to describe the gaseous species; another was used to describe the condensed species.

Because of this distinction, care must be exercised in keeping track of in what state each compound finds itself. At a temperature, T , all compounds whose boiling points are less than or equal to T are gaseous, whereas, all compounds whose boiling points are greater than T are condensed. Consequently, as the temperature of a system varies, the number of condensed species may vary.

A general means of treating this problem is to consider all species, i.e., all phases of all compounds, as being present. Each species would be either gaseous or condensed, and the species could be grouped accordingly. Furthermore, these two groups would remain invariant during the course of the solution, regardless of the temperature and pressure. The physical absence of a given species at a given temperature and pressure should be a natural result of the minimization of the free energy, viz., the given species should have an equilibrium composition of zero moles.

This general method, unfortunately, has certain disadvantages. The number of condensed species would always be unnecessarily large so that the difficulties described in Sections II, C 1 and 2, would be accentuated. To overcome these difficulties, it was shown that certain condensed species must be dropped. Consequently, it seems best to consider only those condensed species which are physically present under a given set of conditions, and reject all those which are physically absent. A second disadvantage is that including all species in the problem, whether they be physically present or not, unnecessarily increases the computer storage and time requirements.

The following scheme was employed to distinguish between the various phases. Since all the possible gaseous species are considered, including the gaseous phase of the condensable species, the phase rule only allows one temperature at which both the liquid and solid phase of any one specie will exist. This temperature is the melting point, and for the purposes of this discussion the normal melting point will be used. At any given temperature there will be present either the solid or the liquid phase of a condensable species and the gaseous phase.

The method proceeds along the following lines: All the compounds are arranged into two groups, the gaseous and those which are condensed.

It is convenient, therefore, to form two matrices at the beginning of a problem: the L_r matrix and the L_u^* matrix. The L_r matrix is composed of rows corresponding to the r always gaseous compounds; it is invariant during the course of the problem. The L_u^* matrix contains two rows for each condensable compound, one row for each of the liquid and solid phases. At a given temperature one row for each compound is taken from the L_u^* matrix and used to form the L_c matrix which characterizes the thermal properties of the condensable compounds at that temperature. The normal melting point of each compound determines which row of L_u^* is to be used in L_c .

The matrix L which characterizes the thermodynamic properties of the entire system is composed of the two submatrices L_r and L_c .

$$\begin{bmatrix} L \end{bmatrix} = \begin{bmatrix} L_r \\ L_c \end{bmatrix} \quad (67)$$

V. THE COMPUTER PROGRAM FOR CALCULATING THE SPECIFIC IMPULSE

A. Flow Diagram for Calculating the Specific Impulse

Figure 2 is a flow diagram which describes both the overall procedure for calculating the specific impulse and the computer program based on this procedure. The overall procedure may be subdivided into three parts:

- (i) Data handling and preliminary calculations
- (ii) Chamber calculation
- (iii) Equilibrium exhaust calculations

Each row of Figure 2 corresponds to one of these parts. Before the methods for calculating temperatures and compositions can be employed, certain data must be available. These data must be selected, retrieved, and calculated, and as is schematically illustrated by the first row of Figure 2. These computer performed operations are discussed below.

1. Read-in Data

Input data consist of the composition mixture, the chamber and exit pressures, a rough estimate of the chamber temperature, and any necessary instructions needed to modify the number of product species considered. (See Appendix II)

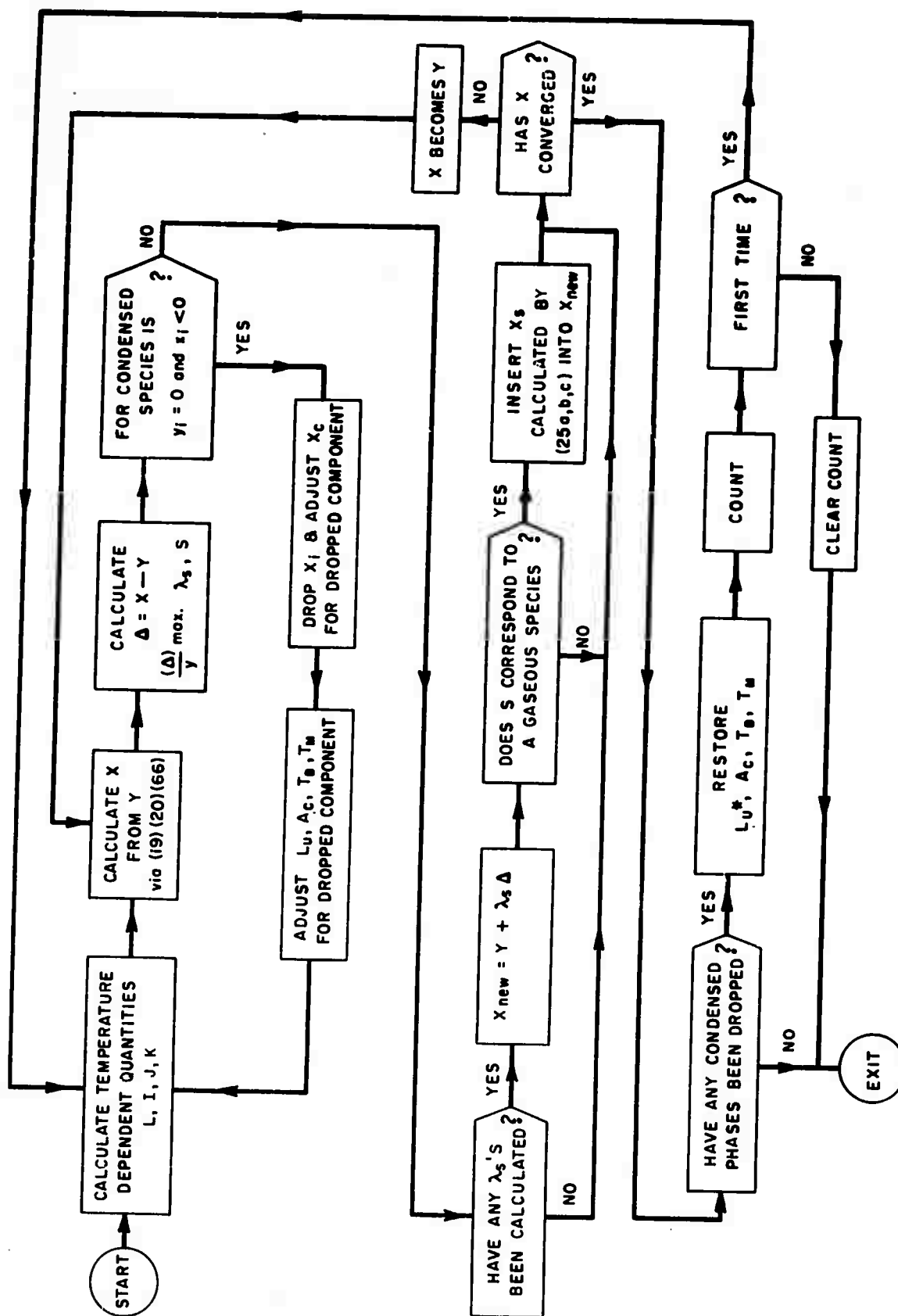


Fig. 2 - Composition Convergence Method

2. What Elements are Present?

A number of predetermined reactants are stored along with their code number, molecular formulas, heats of formation at 298°K., molecular weights, names, and identifying words consisting of the appropriate atomic numbers. This identifying number contains the atomic numbers of all the elements of the compound in ascending numerical order.

3. Construct Reactant Matrices

For each reactant, data are retrieved from the magnetic tape, the A_p and C matrixes are constructed, and a list of each of the following is compiled: molecular weights, heats of formation, and print words for the molecular formulas and names.

4. What Products are Possible?

A number of predetermined products are also stored with their code numbers, formulas, thermodynamic data, molecular weights, melting points, and identifying numbers such as those described for the reactants. Products which contain only those elements present in the fuel mixture are possible species. This is accomplished by comparing the atomic numbers of the elements present, found in part 1 of this discussion, with the atomic numbers in the identifying word. If equality is found, the position of the identifying words in the list is stored as this is the code number of the product.

5. Construct Product Matrices

From the list of code numbers representing the gaseous compounds, the thermodynamic matrix L_r and part of the A matrix are constructed. From the list of code numbers representing the condensed compounds, the thermodynamic matrix L_u^* and the remainder of the A matrix are constructed. A melting point vector T_m and a list of the molecular weights of the products are also constructed.

6. Calculate Percent Composition

In this section the input composition, which can be in either moles or grams, is normalized to 100 g. of propellant by the following method.

$$\text{Define } \rho = \frac{\mu}{\sum_{i=1}^p C_i M_i} \quad (68)$$

where $M = 100$ g.

Then the moles of the i th reactant in the system is:

$$r_i = C_{ip} \quad (69)$$

The mole and weight percent of each reactant are computed at this stage of the process also.

If ΔH_{f_i} is the molar heat of formation of the i th reactant and r_i is the number of moles of the i th reactant, then the enthalpy of the reactant system is:

$$\sum_{i=1}^p r_i \Delta H_{f_i}$$

which is also the enthalpy of the products in the chamber. This quantity is calculated by:

$$\sum_{i=1}^p r_i \Delta H_{f_i} = \rho \sum_{i=1}^p c_i \Delta H_{f_i} \quad (70)$$

To calculate the effects of changes in the heat of formation of the reactants, it is convenient to include two fictitious reactants to the list of propellants. These fictitious reactants have heats of formation of +100 kcal./mole and -100 kcal./mole but no mass. Hence, by including x moles of one of these reactants to a reactant mixture, the heat of formation is increased (or decreased) by $100x$ kcal. and the mass remains unchanged.

7. Store Preliminary Data

The percent composition, formulas and names of the reactants, the formulas of all the products as well as identifying run number are stored on magnetic tape, thereby allowing a large portion of the computer memory to be utilized again.

8. Calculate a Starting Composition

From an element balance the number of gram-atoms of the i th element is given by:

$$b_j = \sum_{i=1}^p a_{ij} r_i \quad (71)$$

where a_{ij} is the number of atoms of element j per molecule of i th reactant. Substitution of equation (69) into (71) gives:

$$b_j = \rho \sum_{i=1}^p a_{ij} r_i \quad (71)$$

where a_{ij} is the number of atoms of element j per molecule of i th reactant. Substitution of equation (69) into (71) gives:

$$b_j = \rho \sum_{i=1}^p a_{ij} c_i \quad (72)$$

or in matrix notation:

$$B = \rho A_p c \quad (73)$$

Consequently, by using equation (73), all the b_j 's, i.e., the gm.-atoms of all the elements in the system, can be calculated at once.

Example:

For the reaction mixture:



1
1 corresponds to N_2H_4
2 corresponds to F_2

1
1 corresponds to H
2 corresponds to N
3 corresponds to F

The formula numbers, a_{ij} , the coefficients of the reaction mixture, c_i , and the molecular weights of the reactants, M_i , are given below.

		H	N	F		
	<u>1</u>	<u>a_{11}</u>	<u>a_{12}</u>	<u>a_{13}</u>	<u>c_1</u>	<u>M_1</u>
N_2H_4	1	4	2	0	1	32.048
F_2	2	0	0	2	2	38.00

From equation (68).

$$\rho = \frac{100.0}{32.048 + 2(38.00)}$$

Equation (73) yields:

$$\begin{bmatrix} B \end{bmatrix} = \rho \begin{bmatrix} 40 \\ 20 \\ 02 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \end{bmatrix} = \rho \begin{bmatrix} 4 \\ 2 \\ 4 \end{bmatrix}$$

that is, the system contains 4ρ gram-atoms of H, 2ρ gram-atoms of N, and 4ρ gram-atoms of F. The total weight of the system is 100 g.

The White, Johnson, Dantzig Method requires a starting composition vector Y which is compatible with the element balance. Let Y^o be an arbitrary Y which will be corrected by Y^c so as to make the resulting Y^* compatible with the element balance:

$$\sum_{i=1}^n a_{ij}y_i^* = b_j \quad (74)$$

Substitution of:

$$y_i^* = y_i^o + y_i^c \quad (75)$$

into (74) produces:

$$\sum_{i=1}^n a_{ij}y_i^o + \sum_{i=1}^n a_{ij}y_i^c = b_j \quad j=1, 2, \dots, m \quad (76)$$

It is desired to determine the y_i^c 's from Equation (76). Since there are but m equations, only m of the y_j 's can be determined from the above equations. Let values of zero, therefore, be assigned to $n-m$ of y_j^c 's so that:

$$\sum_{i=1}^n a_{ij}y_i^o + \sum_{i=1}^m a_{ij}y_i^c = b_j \quad (77)$$

In matrix notation:

$$A' Y^o + A_S' Y^c = B \quad (78)$$

where A_S' is a square $m \times m$ matrix whose columns correspond to m "key" compounds.

Solving (78) for Y^c yields:

$$Y^c = [A_S']^{-1} [B - A'Y^o] \quad (79)$$

where the elements of Y^0 correspond to the m key compounds. From (75) and (79) we obtain:

$$Y = Y^0 + [A_S']^{-1} [B - A'Y^0] \quad (80)$$

where it is understood that the corrections are added only to the y_i^0 's of the key compounds. Hence, given an arbitrary composition vector Y^0 and m key compounds we can calculate a composition vector Y^* which is compatible with the element balance equations.

A convenient choice of Y^0 is a vector each element of which is 0.0001 moles. A convenient choice of key compounds are the chemical elements. This choice of "key compounds" eliminates the possibility of negative y_i^* 's.

White, Johnson, and Dantzig have stated that a suitable starting composition, Y^0 , must satisfy the mass balance constraints, i.e., Equation (7). They also state that round-off errors in the composition introduced during the course of the calculations can be reduced by using an equation similar to (8). These remarks suggest that compositions which are not compatible with the mass balance constraints have a tendency to make the calculated solutions, i.e., X 's, drift from the true solution.

It has been found, however, that the convergence method, at least for a computer with floating point hardware, is self-stabilizing. In other words, the method will seek out the true solution whether the input composition satisfies the mass balance constraints or not. To verify this point the following numerical experiment was performed on a few problems. First, the equilibrium composition was calculated from a starting composition which agreed with the mass balance constraints. Presumably this equilibrium composition was correct. The same calculation was then repeated except that the starting composition disagreed drastically with the mass balance equations. The equilibrium composition calculated in the second case agreed with the correct equilibrium composition.

Therefore, finding a starting composition which is compatible with the mass balance constraints seems to be an unnecessary operation, although composition convergence is attained much faster if a "correct" starting composition is used.

9. Chamber and Exhaust Solutions

The methods used to obtain both the chamber and exhaust solutions have been extensively discussed in Sections II and III. Figure 2 represents a flow diagram of the method used for computing an equilibrium composition.

10. Storing of Results

All results are stored on magnetic tape as they are obtained. After the problem has been completed, a separate program takes the data from the tape and prints the results. Since the program is automatic, this method of storing the solution saves time by the nature of the speed of writing on magnetic tape versus punching out the answers. A sample output is included in Appendix II.

B. Capabilities of the Computer Program

A program for the Burroughs 220 to calculate the specific impulse has been written according to the method illustrated in Figure 3. The capabilities of this program will now be considered.

A study of Figure 2 reveals that the last operation of a given problem reads in the succeeding problem thereby making the program automatic. Any number of problems may be run without manual intervention. Probable error stops and non-converging solutions are accounted for by a printout, which identifies the difficulty, followed by an instruction to read in the next problem. This scheme enables unattended overnight operation of the program.

Provided that sufficient thermodynamic data are available, the program is general. Computer storage capacity, however, imposes certain restrictions on the size of systems that can be treated. These restrictions are:

- (a) 14 or less reactants in the fuel mixture.
- (b) 12 or less elements in the fuel.
- (c) 12 or less condensed species present in the products or reaction.
- (d) 90 or less products of reaction.

To date all of the problems attempted (over 6000) have remained within these restrictions.

The computer time required to solve one complete problem varies from 3 minutes, for simpler problems, to about 50 minutes for the most difficult problems. Most problems average about 25 minutes of computer time.

Input data for a given problem are kept to a minimum. The selection and preparation of thermodynamic data, as well as all preliminary calculations (such as calculating the gram-atoms of each element in the fuel and enthalpy of the fuel) are performed by the computer. The only input data required are the composition of the reaction mixture, the pressures of the chamber and

nozzle exit, and a rough estimate of the chamber temperature. All other pertinent data are retrieved from magnetic tape where they are permanently stored. The composition of the reaction mixture may be entered either in terms of the fuel compounds (which is usually most desirable), or in terms of the elements and the fuel enthalpy.

An example of input and output from the computer is given in Appendix III.

VI. NOMENCLATURE

A	- an $m \times n$ matrix whose elements are a_{ij} for the n products of combustion.
A_c	- an $m \times n_c$ matrix whose elements are a_{ij} for the n_c condensed products of combustion.
A_g	- an $m \times n_g$ matrix whose elements are a_{ij} for the n_g gaseous products of combustion.
A_p	- an $m \times p$ matrix whose elements are a_{ij} for the p propellants.
A_s	- an $m \times m$ matrix whose elements are a_{ij} for the m "key" components used in making a mass balance.
B	- an $m \times 1$ column matrix whose elements are b_j .
$C_p(T)$	- the heat capacity at constant pressure as a function of temperature.
C_{pi}	- the heat capacity at constant pressure at the temperature T_i , cal./mole/°K.
F_i	- the free energy of the i th species, cal./mole.
$F(T)$	- the molar free energy of a compound as a function of temperature, in cal.
$F_r(X)$	- the free energy of a system at a given temperature as a function of the composition X divided by RT .
\mathcal{F}	- an $n \times 1$ column matrix whose elements are \mathcal{F}_i .
\mathcal{F}_c	- an $n_c \times 1$ column matrix whose elements are the \mathcal{F}_i for the condensed species.
\mathcal{F}_i	- the ideal partial molal free energy of the i th species divided by RT .
\mathcal{F}_g	- an $n_g \times 1$ column matrix whose elements are the \mathcal{F}_i for the n_g gaseous species.
G	- a function defined by Equation (8).
$H(T)$	- the enthalpy of the system as a function of temperature, in cal.

- $H(T, X)$ - the enthalpy of the system as a function of temperature and composition, in cal.
- $H(T, X, P)$ - the enthalpy of the system as a function of temperature composition and pressure, in cal.
- H_c - the enthalpy of μ grams of products in the rocket chamber, in cal.
- H_e - the enthalpy of μ grams of products at the rocket exit, in cal.
- $H_E(T^\circ)$ - the enthalpy of the elements at the reference temperature, cal./mole.
- H_i - the molar enthalpy of the i th species, in cal./mole.
- H_n - the enthalpy of the system calculated at the temperature, T_n , in cal.
- ΔH_{fj} - the heat of formation at the reactant temperature of the j th reactant, in cal./mole.
- I - the column matrix corresponding to \vec{I} .
- I_j - a function of temperature which is used to describe the enthalpy of a system, units depend on j .
- \vec{I} - the enthalpy thermal vector; a vector whose elements are I_j .
- I_{sp} - the specific impulse, in seconds.
- J_j - a function of temperature which is used to describe the entropy of a system, units depend on j .
- J - the column matrix corresponding to \vec{J} .
- \vec{J} - the entropy thermal vector; a vector whose elements are J_j .
- K - the column matrix corresponding to \vec{K} .
- K^* - K/RT
- K_j - a function of temperature which is used to describe the free energy of a system, units depend on j .

\vec{K}	- the free energy thermal vector; a vector whose elements are K_j .
L	- an $n \times (N+2)$ matrix known as the thermodynamic property matrix; its rows are the \vec{I} 's for all the compounds in the system at a given temperature.
L_c	- an $n_c \times (N+2)$ matrix; its rows are the \vec{I} 's for the n_c condensed species at a given temperature.
L_u^*	- a $3u \times (N+2)$ matrix; its rows are <u>all</u> of the \vec{I} 's for the u condensable compounds.
L_r	- a $r \times (N+2)$ matrix; its rows are the \vec{I} 's for the always gaseous compounds.
L_g	- an $n_g \times (N+2)$ matrix; its rows are the \vec{I} 's for the n_g gaseous compounds at a given temperature.
M_i	- the molecular weight of the i th species, gm./mole.
M	- an $n \times 1$ column matrix whose elements are M_i .
N	- the number of terms used to characterize the functional dependence of C_p with temperature.
P	- the pressure of the system, in atm.
P_e	- the pressure at the nozzle exit, in atm.
P_c	- the pressure in the rocket chamber, in atm.
P	- an $n \times 1$ column matrix whose elements are P_i .
P_i	- the ideal entropy of mixing of the i th species divided by R .
P_c	- an $n_c \times 1$ column matrix whose elements are the entropy of mixing of the n_c condensed species divided by R . This matrix is null.
P_g	- an $n_g \times 1$ column matrix whose elements are the P_i for n_g gaseous species.

$Q(X)$	- the quadratic approximation to the free energy resulting from a Taylor's Expansion of $F(X)$.
R	- the gas constant per mole, cal./mole/°K.
$S(T,X,P)$	- the entropy of the system as a function of temperature, composition, and pressure, in e.u.
S_i	- the molar entropy of the i th product species, in e.u.
\bar{S}_i	- the partial molar enthalpy of the i th product species, in e.u.
S_c	- the entropy of μ grams of products in the rocket chamber, in e.u.
ΔS_i	- the ideal entropy of mixing of the i th product species, in e.u.
T	- the temperature, °K.
T_n	- the n th approximation to a solution temperature.
T_b	- a base temperature, °K.
T°	- the reference temperature, °K.
X	- an $n \times 1$ vector whose components are x_i .
X_c	- an $n_c \times 1$ column matrix whose components are the x_i for the n_c condensed species.
X_c°	- the equilibrium X at the chamber temperature.
X_e	- the X of the product species at the rocket exit.
X_e°	- the equilibrium X at the rocket exit temperature for equilibrium flow.
X_g	- a $n_g \times 1$ column matrix whose elements are the x_i for the n_g gaseous species.
X_{new}	- $Y + \lambda \Delta$
Y	- an $n \times 1$ column matrix whose components are the y_i .
Y^*	- an $n \times 1$ column matrix whose components, y_i^* , satisfy the mass balance constraints.

- y^o - an arbitrary $n \times 1$ column matrix whose elements are y_1^o .
- y^c - an $n \times 1$ column matrix whose components are y_1^c .
- y_g - an $n_g \times 1$ column matrix whose elements are the y_1 for the n_g gaseous species.
- y_{gD} - an $n_g \times n_g$ diagonal matrix whose diagonal elements are the y_1 for the n_g gaseous species.

- a - an empirical constant used to describe heat capacity data.
- \vec{a}_i - the formula designation vector; a vector whose elements are $a_{i1}, a_{i2}, \dots, a_{im}$.
- a_{ij} - a formula designation number which indicates the number of atoms of element j in a molecule of species i .
- b - an empirical constant.
- b_j - the total number of gm. atomic weights of element j present in the mixture.
- c - a constant; in Equation (1) $c = 9.3281 \frac{\text{gm.}^{1/2}}{\text{kcal.}} \text{ sec.}$
- c_i - the number of moles of the i th reactant in the reaction mixture (propellant).
- $c(T)$ - the number of condensed compounds in a given system at the temperature T .
- d - a constant.
- e - a constant.
- $f_j(T)$ - a function of temperature used to describe constant pressure heat capacity data.
- l_j - empirical constant used to describe thermodynamic properties, see Equations 36, 43 and 44.
- \vec{l} - a thermodynamic property vector; a vector whose elements are l_j .
- m - the number of chemical elements in a given system.

- n - the total number of product species of a system.
- n_c - the number of condensed product species of the system at a given temperature.
- n_g - the number of gaseous product species of the system at a given temperature.
- p - the number of reactants (propellants).
- r - the number of compounds in a given system which are always gaseous above 1000°K.
- r_j - the number of moles of the j th reactant in the propellant mixture.
- u - the number of condensable compounds in a given system.
- $v(T)$ - the number of vaporized compounds in a given system at the temperature T .
- \bar{x} - the summation of the gaseous x_i .
- $\frac{\bar{x}}{\bar{y}}$ - an $n_g \times 1$ column matrix whose elements are all \bar{x}/\bar{y} .
- x_c - the corrected value of \bar{x} given by (26).
- x_i - the number of moles of the i th product species; x_i is a variable.
- x_s - the number of moles of the s th product species where s identifies the smallest λ , (see Equation 24).
- y_s - the y_i which corresponds to x_s .
- \bar{y} - the summation of the gaseous y_i .
- y_i - the number of moles of the i th product species; y_i is one of the coordinates of Y , a fixed point about which a Taylor's Expansion is made.
- y_i^* - the number of moles of the i th species; an element of Y^* .
- y_i° - an arbitrary number of moles of the i th species.
- y_i^c - $y_i^* - y_i^\circ$.

- α - an $m \times 1$ column matrix whose elements are α_j .
- α_j - the atomic weight of the j th element.
- λ - a scale factor which reduces the step length given by Δ . See Equation (23).
- λ_1 - the largest λ which prevents x_1 from becoming negative.
- λ_s - the smallest of all the λ_1 .
- μ - the mass of the propellant system, in gms.
- π - an $m \times 1$ vector whose elements are the π_j 's.
- π_j - a Lagrange multiplier associated with the mass balance equation for the j th element.
- $\vec{\pi}$ - a vector whose elements are the π_j .
- ρ - the number of reaction weights in a system of mass μ .
- σ_k - a constant multiplier.
- ϕ_H - a factor used in estimating improved temperatures when enthalpy is used in the convergence criterion.
- ϕ_s - a factor used in estimating improved temperatures when entropy is used in the convergence criterion.
- Δ - an $n \times 1$ column matrix or vector which indicates the directions toward an improved solution $X-Y$.
- Δ_i - an element of Δ , $x_1 - y_1$.

Subscripts

- c - chamber conditions; condensed species.
- e - exit conditions.
- g - gaseous species.
- i - a dummy index usually used to designate a species.
- j - a dummy index usually used to designate a chemical element.

k - a dummy index.

Superscripts

$'$ - denotes the transpose of a matrix.

-1 - denotes the inverse of a matrix.

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VIII. APPENDICES

APPENDIX I

THE THERMODYNAMIC PROPERTY VECTORS OF THE COMBUSTION PRODUCTS

The general formulation of the thermodynamic property vectors given in Section IV is now applied using the heat capacity expression suggested by Thomson⁴ and the thermodynamic property data compiled by The Dow Thermal Laboratory.⁶ The thermodynamic property vectors resulting from the above source are tabulated at the end of this Appendix.

The constant pressure heat capacity expression proposed by Thomson is of the form:

$$C_p = l_1 + l_2 + l_3 T^2 + l_4 T^3 + l_5 T^{-2} \quad (81)$$

where T is the temperature in °K., divided by 1000 and the l_i 's are constants to be determined from experimental measurements.

Following the method prescribed by Thomson, the constants l_1 through l_5 were calculated from values of the heat capacity measured at five characteristic temperatures. If T_1 to T_5 and C_{p1} to C_{p5} are the characteristic temperatures and their corresponding heat capacities, respectively, then (81) leads to the following matrix equation:

$$\begin{bmatrix} C_{p1} \\ C_{p2} \\ C_{p3} \\ C_{p4} \\ C_{p5} \end{bmatrix} = \begin{bmatrix} 1 & T_1 & T_1^2 & T_1^3 & T_1^{-2} \\ 1 & T_2 & T_2^2 & T_2^3 & T_2^{-2} \\ 1 & T_3 & T_3^2 & T_3^3 & T_3^{-2} \\ 1 & T_4 & T_4^2 & T_4^3 & T_4^{-2} \\ 1 & T_5 & T_5^2 & T_5^3 & T_5^{-2} \end{bmatrix} \begin{bmatrix} l_1 \\ l_2 \\ l_3 \\ l_4 \\ l_5 \end{bmatrix} \quad (82)$$

Solving for unknowns l_i 's gives:

$$\begin{bmatrix} l_1 \\ l_2 \\ l_3 \\ l_4 \\ l_5 \end{bmatrix} = \begin{bmatrix} \tau \end{bmatrix}^{-1} \begin{bmatrix} C_{p1} \\ C_{p2} \\ C_{p3} \\ C_{p4} \\ C_{p5} \end{bmatrix} \quad (83)$$

where τ is the square matrix of Equation (82). For species not undergoing phase changes, the five characteristic temperatures are:

1000, 1600, 3000, 4500, and 5700°K.

However, if a phase change did occur, then five temperatures with spacings proportional to those above were chosen so as to cover the complete temperature range of each phase. (Table III contains the temperature range used in calculating the l_1 's for each compound.) Equation (83), therefore, is used to calculate l_1 through l_5 .

The quantities l_6 and l_7 are calculated according to (43a) and (44a):

$$l_6 = H(T_b) - \sum_{j=1}^5 l_j I_j(T_b) \quad (43a)$$

$$l_7 = S(T_b) - \sum_{j=1}^5 l_j J_j(T_b) \quad (44a)$$

Before these expressions can be applied, the functions H , S , I , and J must be evaluated at $T = T_b$.

Absolute entropies are generally obtainable, but absolute enthalpies are not.* Consequently, $S(T_b)$, in (44a), is the absolute entropy at the base temperature, T_b , while $H(T_b)$, in (43a), must be a relative enthalpy. A convenient reference state for evaluating enthalpies is the elements at standard conditions. If this reference state is chosen then:

$$H(T_b) = [H(T_b) - H(T^\circ)] + [H(T^\circ) - H_E(T^\circ)] \quad (74)$$

Both of the bracketed terms on the right side of (74) are available from the Thermodynamic Tables⁶. The first term is the change in enthalpy in going from the reference temperature, T° , to the base temperature, T_b , while the second term is the heat of formation from the elements at T° . The entropy at the base temperature, $S(T_b)$, is also available from the Thermodynamic Tables.⁶

The functions I and J are defined by Equations (39) and (40).

$$I_j(T) = \int f_j(T) dT \quad (39)$$

$$J_j(T) = \int \frac{f_j(T)}{T} dT \quad (40)$$

The above integrations are straightforward and are given in Table II.

* This stems from difficulties in measuring the zero point energy.

† This reference state is especially useful in treating multi-component systems since it is independent of the composition.

TABLE II
Elements of the Thermal Vectors

J	$f_j(T)$	$I_j(T)$	$J_j(T)$	$K_j(T)$
1	1	T	$\ln T$	$T(1 - \ln T)$
2	T	$1/2 T^2$	T	$- 1/2 T^2$
3	T^2	$1/3 T^3$	$1/2 T^2$	$- 1/6 T^3$
4	T^3	$1/4 T^4$	$1/3 T^3$	$- 1/12 T^4$
5	T^{-2}	$-T^{-1}$	$- 1/2 T^{-2}$	$- 3/2 T^{-1}$
6	-	1	0	1
7	-	0	1	-T

Hence, from $H(T_b)$ calculated via (84), $S(T_b)$ obtained from the Thermodynamic Tables⁶, and $I_j(T_b)$ and $J_j(T_b)$ calculated from Table II, l_6 and l_7 can be evaluated using (43a) and (44a).

Study of Equation (31) or (32) reveals that T_b must be chosen within the temperature range for which l_1 through l_5 are valid. Choosing a T_b outside this range is satisfactory only if l_1 through l_5 represent the behavior of C_p versus T to the temperature T_b . This condition, however, does not generally prevail. Because of slight variations between the observed heat capacity data and those predicted from l_1 through l_5 , slight variations in l_6 and l_7 occur if T_b is allowed to vary. Therefore, rather than choose l_6 and l_7 corresponding to a given T_b , it seems best to calculate the average values of l_6 and l_7 based on several T_b 's. Values of l_6 and l_7 entered in Table III are the arithmetic means of l_6 and l_7 calculated at T_b 's equal to the five characteristic temperatures described above.

By itself the thermodynamic property vector l has little significance; it must be associated with the enthalpy thermal vector, I , the entropy thermal vector, J , or the free energy thermal vector, K , before it takes on real significance. The elements of these thermal vectors are listed in Table II. Notice that f_1 through f_5 are defined by (81), I_j and J_j for $j=6$ and 7 are defined by (43) and (44) and the K_j 's are defined by (48).

Using the procedure outlined above, the elements (l_1 through l_7) of the thermodynamic property vectors of 98 combustion products have been calculated. The results of these calculations are entered in Table III below.

Values of C_p , H , and S generated from the thermodynamic property vectors in Table III agree with the tabulated values⁶ to better than 1 per cent.

TABLE III
The Thermodynamic Property Vectors of the Combustion Products

Compound	State	11, cal. mole ⁻¹ deg. ⁻¹	12, cal. mole ⁻¹ deg. ⁻²	13, cal. mole ⁻¹ deg. ⁻³	14, cal. mole ⁻¹ deg. ⁻⁴	15, cal. mole ⁻¹ deg.	16, cal. mole ⁻¹	17, cal. mole ⁻¹ deg.
H ₂	Gas	5.744149	1.635989	-.248476	.016153	.072174	-1.448891	38.230614
I ₂	Gas	2.457282	1.640946	-.429339	.055169	2.002388	40.618854	38.573728
	Liquid	-2.418100	14.759800	-8.659400	1.747200	1.440980	4.451267	6.252690
Be	Gas	5.699850	-.533923	.075088	.010273	-.281289	75.642194	28.908278
	Liquid	7.502100	-.001300	.000180	-.000033	-.000300	-.951992	10.374975
	Solid	-11.240600	28.868500	-16.846900	3.763280	1.985610	7.375959	-11.981354
B	Gas	4.835241	.138751	-.049714	.005982	.039740	132.830600	42.564206
	Liquid	7.500060	-.000030	.000001	-.000001	-.000110	.130018	8.229363
	Solid	6.307720	.276890	.150950	-.007161	-.829511	-4.083669	5.832890
C	Gas	4.955040	-.115265	.088130	-.008817	.050912	169.491920	43.876216
	Solid	5.952581	.090093	.047530	-.004650	-.945554	-4.137887	5.266828
N ₂	Gas	7.929263	.590846	-.108108	.007366	-.609376	-3.671440	53.670058
O ₂	Gas	7.801681	.736242	-.044413	-.001623	-.151897	-2.883333	57.408590
F ₂	Gas	8.917622	.170069	.002042	-.000356	-.239384	-3.363328	58.142316
Na	Gas	5.457544	-.261398	-.022043	.023565	-.263275	23.800082	42.863912
	Liquid	14.614400	-18.224200	14.797300	-3.853600	-.405500	-4.285798	34.428566
Mg	Gas	6.563759	-1.000133	.148239	.008449	-.994329	31.998536	41.963526
	Liquid	5.259000	2.600000	-.011000	.001000	-.001000	.456393	15.704905
Al	Gas	2.228060	1.673550	-.392364	.033841	3.088500	80.624890	45.009532
	Liquid	6.999970	-.000020	-.000010	.000002	.000021	.350119	17.525313
Si	Gas	3.585831	1.187848	-.244481	.016644	.464157	104.928180	45.462232
	Liquid	7.000032	-.000014	.000003	-.000000	-.000020	7.959939	17.816459
	Solid	4.009400	2.841300	-.874300	.124770	-.240270	-.816493	9.073350
P	Gas	4.317574	.141874	-.027145	.002034	-.034338	19.913882	30.959438

TABLE III (cont'd.)

Compound	State	11, -1 cal. mole deg.	12, -1 cal. mole deg.	13, -1 cal. mole deg.	14, -1 cal. mole deg.	15, -1 cal. mole deg.	16, -1 cal. mole deg.	17, -1 cal. mole deg.
S	Gas	4.439339	.059446	-.007343	.000603	-.072050	13.459281	32.248750
Cl ₂	Gas	8.981033	.091746	.008968	-.000872	-.120880	-3.048689	63.580914
AlCl	Gas	9.005823	.053504	.012649	-.001072	-.100901	-14.566059	64.855124
AlCl ₃	Gas	20.160797	-.238597	.062530	-.005176	-.429443	-145.569220	98.359028
AlF	Gas	8.897665	.099776	.001728	-.000469	-.178698	-63.703382	61.305636
AlF ₃	Gas	19.780051	.062389	-.015328	.001297	-.578400	-291.450500	87.277874
	Solid	20.944700	2.971400	.013900	-.003300	-.000800	-362.204500	39.626656
AlH	Gas	8.631479	.336546	-.034554	.002323	-.565797	57.754178	53.-01928
Al ₂ O	Gas	13.578075	.183637	-.036000	.002276	-.867991	-43.333574	73.707984
AlO	Gas	8.950356	.055608	.010295	-.001042	-.285214	12.436627	61.797460
Al ₂ O ₃	Liquid	34.999000	.000600	-.000100	.000010	.001400	-794.488800	51.719042
	Solid	30.368400	-1.342800	2.257200	-.385520	-1.098570	-413.211740	49.870188
B ₂	Gas	8.931215	.099802	.002568	-.000289	-.323256	198.950980	57.767184
BCl	Gas	8.945361	.086346	.001781	-.000208	-.223274	41.487148	60.771380
BCl ₃	Gas	19.766962	.063183	-.014245	.001120	-.707035	-105.081510	90.048176
BF	Gas	8.686775	.225412	-.031870	.002250	-.422567	-46.856898	56.800514
BF ₃	Gas	19.335961	.316310	-.066960	.004814	-1.460134	-276.604480	78.350340
BH	Gas	7.974582	.678720	-.111491	.007834	-.709645	112.331420	48.823448
BN	Gas	8.619241	.269865	-.048039	.004308	-.475376	150.534480	58.995974
	Solid	11.079684	.871314	-.200260	.026036	-1.231697	-67.113745	11.657738
B ₂ O ₂	Gas	19.879683	.534709	-.109022	.007902	-1.583249	-114.739980	78.260484
BO	Gas	8.419721	.349223	-.055905	.004854	-.587894	6.870053	56.958908

APPENDIX II

INPUT

Input data for a given problem consist of:

- (i) A test word which indicates whether the input is in moles or grams, and whether a modification in the number of product species is to be considered.
- (ii) The propellant composition designated by two numbers. The first number is the number of moles or grams of the given reactant in the reaction mixture and the second number identifies the reactant.
- (iii) The chamber and exit pressures.
- (iv) A rough estimate of the chamber temperature.
- (v) An identifying run number.
- (vi) Any appropriate changes in the melting points of the condensable species.
- (vii) Any modification of the product species.

Figure 3 is a sample input sheet for a lithium aluminum hydride-nitronium perchlorate- polyethylene system. The pressures and temperature are given in floating decimal number.

There is also included the output data sheet obtained from the input (Figure 4).

Fig. 3 - Sample Input for Specific Impulse Calculation

		10				
18.00			.0685			
62.00			.0620			
20.00			.0562			
.				02		
.						
.						
.						
.						
.				03		
.						
.						
.						
.						
.				04		
.						
52 68	04	57 00				
51 10	00					
54 30						
				05		
6	04	51 38				
				06		
				6a		

Test word

Fuels

Product

Selection

P_c
 P_e
 T_c
 Run No.

Melting Point Change

6	30	0495	-
			8

6		04	4956	
				7
				7a
				7b
				7c
				7d
				7e

Run Number 5736

No. Products 58 No. Gases 54 No. Condensed Phases 4

Percent		Formula	Name	ΔF_{298}°
Mole	Weight			
29.40	18.00	LiAlH ₄ -s	Lithium Aluminum Hydride	
26.42	62.00	ClNO ₆ -s	Nitronium Perchlorate	
44.19	20.00	C ₂ H ₄ -s	Polyethylene	

Species	Chamber Moles	Exhaust Moles	Exhaust Grams
Al	.001737		
AlCl	.010421		
AlClO	.000019		
AlCl ₂	.003354		.000001
AlCl ₃	.000008		
AlH	.000438		
AlHO	.000021		
AlHO ₂	.001975		
AlN	.000001		
AlO	.000635		
Al ₂ O	.002284		
Al ₂ O ₂	.000022		
HCN	.000156	.000003	.000086
CHNO	.000007		.000005
CHO	.001283	.000009	.000264
CH ₂ O	.000021		.000012
CH ₄	.000002		.000007
CN	.000006		
CO	1.394454	1.370447	38.387588
CO ₂	.029877	.055330	2.435122
Cl	.003279	.000003	.000101
HCl	.075704	.008211	.299418
HOCl	.000001		
LiCl	.328966	.402002	17.043689
Cl ₂	.000001		
Li ₂ Cl ₂	.000544	.007995	.677887
Li ₃ Cl ₃		.000002	.000208
H	.123172	.000919	.000926
LiH	.009217	.000107	.000850
LiOH	.082462	.054228	1.298659

Fig. 4 - Output Data Sheet
-46-

Run Number 5736 (Continued)

Species	Chamber Moles	Exhaust Moles	Exhaust Grams
NH	.000037		
OH	.008881	.000009	.000156
H ₂	1.897070	2.032152	4.096817
H ₂ O	.325619	.310483	5.593658
Li	.048864	.001925	.013361
LiN	.003041	.000016	.000333
LiO	.000422		.000004
Li ₂ O	.000108	.000002	.000064
N	.000008		
NO	.000361		.000002
N ₂	.211302	.213100	5.970205
O	.000333		
O ₂	.000023		
Al ₂ O ₃ -s, l	.225530	.237142	24.178961

Temperature, °K.	3278.838	1781.701
Pressure, atmos.	68.046	1.000
Enthalpy, kcal.	-17.288	-113.398
Entropy, e.u.	267.536	267.542
Moles of gas	4.566	4.457
Avg. mol. wt., g.	16.864	17.011
Gamma	1.271	1.297
Velocity, cm./sec.		283601.740
Impulse, sec.		289.182

Fig. 4 (Contd.)

Appendix III

Constants for the Generation of Thermodynamic Properties

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
1 Al-s,1							
Liquid	.313024	6.999998		-.000002			17.505829
Solid	-1.405771	4.509173	3.726023	-.395728	.056896	.030096	11.293808
2 Al							
Gas	76.676926	4.776660	.251993	-.105005	.013815	.034967	45.190472
3 AlCl							
Gas	207.166560	8.936989	.003666	-.000649	.000029	-.036166	64.836556
4 AlCl							
Gas	-14.515948	8.927057	.128628	-.002432	.000183	-.069447	64.650664
5 AlClF							
Gas	-127.842500	13.822715	.058575	-.013266	.000989	-.221203	83.207030
6 AlClF ₂							
Gas	-242.387820	19.654005	.143912	-.032649	.002457	-.470776	92.167426
7 AlClO							
Gas	-60.434504	14.743334	.106130	-.034068	.001806	-.319903	75.605400
8 AlCl ₂							
Gas	-82.622110	13.873462	.025127	-.005930	.000467	-.146151	85.510600
9 AlCl ₂ F							
Gas	-188.891440	19.741701	.086295	-.019562	.001471	-.369535	95.940084
10 AlCl ₃ -s,1							
Liquid	-171.260020	32.000014	-.000010	.000010	-.000001	-.000002	79.318950
Solid	-175.139200	21.494140	3.303880	-.057440	.002047	.000239	51.684118
11 AlCl ₃							
Gas	-147.229740	19.795746	.052108	-.012092	.000926	-.275726	97.712420

Constants for the Generation of Thermodynamic Properties (Contd.)

	17	11	12	13	14	15	16
12 ALF							
Gas	-64.437528	8.844102	.156476	-.015131	.001147	-.154175	61.262344
13 ALFO							
Gas	-126.894180	14.657329	.162297	-.036673	.002746	-.470914	71.226150
14 ALF ₂							
Gas	-162.176490	13.747689	.106437	-.023870	.001773	-.332791	77.708208
15 ALF ₃ -s							
Solid	-364.485000	23.030046	.472470	1.060943	-.148793	-.435725	41.273244
16 ALF ₃							
Gas	-293.140800	19.512428	.239812	-.054846	.004147	-.595287	85.914286
17 ALH							
Gas	58.548288	8.016235	.759065	-.134423	.010026	-.238854	53.253478
18 ALHO							
Gas	-10.091417	13.521079	.903354	-.203669	.015229	-.822436	63.538370
19 ALHO ₂							
Gas	-115.792090	15.958609	2.337450	-.500433	.036253	-.609940	76.326640
20 LiAlO ₂ -s,1							
Solid	-293.046520	22.057610	2.945100	-.032810	.008017	-.598256	35.181416
21 AlN-s							
Solid	-79.647272	8.885381	4.186307	-.731181	.001142	-.243969	13.168159
22 AlN							
Gas	101.326920	8.816987	.195019	-.019385	.001471	-.167959	64.091422
23 AlNaO ₂							
Solid	-288.517760	36.590060	-23.166150	16.147530	-3.213237	-1.809068	58.656186
24 AlO							
Gas	14.154399	8.752837	.207667	-.028478	.002142	-.195455	61.724172

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
25 AlSi							
Gas	65.998922	8.903370	.120445	-.006091	.000466	-.105032	65.272192
26 Al ₂ Cl ₆							
Gas	-323.176700	43.594463	.082839	-.018824	.001415	-.557589	167.293000
27 Al ₂ MgO ₄							
Solid	-550.545980	36.811190	6.383990	.007240	-.000937	-.979208	56.402300
28 Al ₂ O							
Gas	-44.902828	13.488140	.280113	-.063833	.004813	-.463210	75.546296
29 Al ₂ O ₂							
Gas	-113.545420	20.093349	.506919	-.114507	.008572	-.709317	82.241378
30 Al ₂ O ₃ -s,1							
Liquid	-353.572260	-2.954006	33.937299	-9.912413	.942705	1.186401	27.576094
Solid	-412.873800	28.590178	3.510837	-1.250880	.140219	-1.176349	39.578596
31 Al ₂ O ₅ Si							
Solid	-669.998620	40.055870	5.926070	-.043380	.009098	-1.010293	63.987954
32 Al ₄ C ₃							
Solid	-65.339212	43.665350	3.372740	-.071990	.008985	-1.063709	70.848058
33 B-s,1							
Liquid	-.333478	7.265811	.300591	-.088045	.007555	-.574260	8.138727
Solid	-2.203576	4.282623	2.819016	-.798698	.078112	-.251056	4.450282
34 B							
Gas	131.172050	4.910933	.076806	-.033186	.004591	.006847	42.603302
35 BCl							
Gas	40.062010	8.830411	.167809	-.016775	.001259	-.165320	60.735858
36 BClF							
Gas	-83.213296	13.087646	.539613	-.122070	.009154	-.475521	76.643810

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
37 BClF ₂							
Gas	-219.840100	18.740476	.739276	-.166538	.012439	-.814008	84.473538
38 BOC1							
Gas	-90.087446	13.599501	.838962	-.187430	.013935	-.376467	71.417936
39 BCl ₂							
Gas	-24.610648	13.720012	.125898	-.028470	.002127	-.279028	80.550048
40 BCl ₂ F							
Gas	-161.836720	19.130728	.487693	-.110449	.008287	-.674250	88.337232
41 BCl ₃							
Gas	-104.704350	19.489910	.252036	-.057133	.004287	-.556545	89.964366
42 BF							
Gas	-48.737594	8.357616	.455160	-.086278	.006462	-.245859	56.710808
43 BOF							
Gas	-148.585490	13.407415	.965814	-.216333	.016119	-.516564	67.573500
44 BF ₂							
Gas	-139.321510	13.117458	.519330	-.117390	.008799	-.492219	72.376776
45 BF ₃							
Gas	-278.449440	18.336059	1.004078	-.226506	.016943	-.934649	77.990752
46 BH							
Gas	112.239560	6.995424	1.367169	-.270654	.019985	-.126461	48.570182
47 BOH							
Gas	-52.515988	11.617090	2.095887	-.466533	.034635	-.590683	59.193072
48 HOBO							
Gas	-141.994860	13.915040	3.582615	-.770552	.055989	-.763678	69.387450

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
49	BH ₂						
Gas	61.436400	10.084665	2.429497	-539523	.039996	-.474133	56.511172
50	BH ₂ O ₂						
Gas	-53.721498	18.347725	4.530856	-.977580	.071147	-.973413	79.036864
51	BH ₃						
Gas	12.700039	10.020179	6.105641	-1.336416	.098161	-.675542	52.164544
52	H ₃ BO ₃						
Gas	-251.814180	26.146019	7.053549	-1.525544	.111213	-1.631083	87.711906
53	NaBH ₄ -s,1						
Solid	-67.409946	47.485580	-31.931620	19.944650	-4.097810	-2.915957	76.437216
54	BN-s						
Solid	-66.851758	11.261024	.598636	-.100663	.006426	-1.023995	12.186024
55	BN						
Gas	148.521330	8.217233	.546445	-.106420	.007949	-.245461	59.350364
56	NaBO ₂ -s,1						
Liquid	-240.046300	28.409067	1.153760	-.473244	.065541	-1.140955	46.623770
Solid	-237.080920	11.600070	13.999840	.000050	-.000059	-.000006	27.433676
57	BO						
Gas	.796945	7.660478	.866139	-.183943	.013690	-.206819	56.693806
58	BS						
Gas	67.207352	8.590891	.287221	-.052261	.003909	-.230482	60.842274
59	B ₂						
Gas	196.030040	8.699155	.262340	-.035955	.002679	-.211418	57.636122

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
60	B_2Cl_4						
Gas	-130.449870	30.141483	.436143	-.098996	.007437	-.918935	117.122610
61	B_2H_6						
Gas	-10.268054	27.946382	9.983782	-2.212206	.163718	-2.914923	72.329126
62	B_2O_2						
Gas	-119.563840	18.029968	1.823048	-.407451	.030310	-.799606	74.653442
63	$B_2O_3-s,1$						
Liquid	-318.104840	33.376392	-1.272985	.373093	-.031186	-2.782318	48.006302
Solid	-280.626320	-65.924870	199.075130	-127.073663	26.734663	3.953444	-100.183890
64	B_2O_3						
Gas	-221.311840	21.347133	2.892342	-.647421	.048203	-1.513369	82.007612
65	$B_3Cl_3O_3$						
Gas	-423.214480	47.357105	1.525525	-.344919	.025838	-2.209970	129.124690
66	$B_3F_3O_3$						
Gas	-589.178280	46.963580	1.786232	-.404218	.030296	-2.553608	121.858300
67	$B_3H_3O_3$						
Gas	-568.137380	54.494210	7.814724	-1.674013	.121297	-3.103061	130.900150
68	$B_3H_3N_3$						
Gas	-150.314570	45.215270	13.729205	-2.989808	.218921	-3.845194	100.866120
69	$B_4C-s,1$						
Liquid	-1.900567	29.510904	.421625	-.121948	.010631	-1.232141	41.224142
Solid	-25.487032	25.540513	6.263060	-2.722480	.376390	-1.709618	26.876722
70	$Na_2B_4O_7-s,1$						
Liquid	-827.583020	87.553550	4.229260	-1.300350	.134505	-5.830977	121.215510
Solid	-797.655320	27.099780	57.999800	-.000200	-.000030	.000005	60.807426

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
71	BsHs						
Gas	-20.670278	55.509220	15.255991	-3.390231	.251344	-5.938271	99.917626
72	BrCH ₁₄						
Gas	-60.494198	103.348080	22.743120	-5.053538	.374644	-10.065773	153.632870
73	Be-s,1						
Liquid	1.098488	4.766792	2.244073	-.568624	.045512	-.388090	8.742361
Solid	-1.725879	4.607906	1.724538	.340273	-.061700	-.072130	6.833384
74	Be						
Gas	76.394542	5.018807	.013976	-.068346	.022217	-.010871	38.568546
75	BeC ₂						
Gas	128.889160	12.332072	1.644152	-.366160	.027173	-.758501	61.367740
76	BeCl						
Gas	33.818630	8.829016	.168060	-.016974	.001273	-.166241	61.694032
77	BeClF						
Gas	-130.262980	14.360690	.356315	-.080378	.006009	-.617626	70.078278
78	BeCl ₂						
Gas	-86.033954	14.581060	.213180	-.048439	.003645	-.405249	73.367652
79	BeF						
Gas	1.525062	8.511206	.362150	-.064690	.004874	-.237679	58.203498
80	BeF ₂						
Gas	-189.168040	13.905903	.652467	-.147193	.011014	-.695429	65.498250
81	BeH						
Gas	74.533868	7.460431	1.088219	-.209795	.015539	-.187259	50.111682

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
82	BeHO						
Gas	-44.952074	9.334943	2.682100	-.567772	.040837	-.344789	62.190978
83	BeH ₂						
Gas	23.836242	11.289797	2.327007	-.520486	.038733	-.880755	50.237890
84	BeH ₂ O ₂						
Gas	-165.684580	16.141763	6.386887	-1.368356	.099171	-1.261378	64.896484
85	BeO-s,1						
Liquid	-127.925810	-.791018	12.844814	-3.135429	.245308	.530452	8.255100
Solid	-148.287520	10.726526	2.133544	-.550426	.054482	-.588126	12.655268
86	BeO						
Gas	27.199116	8.261933	.512788	-.100278	.007515	-.246050	55.903880
87	Be ₂ C						
Liquid	-12.348956	19.500016	-.000024	-.000002		-.000001	28.569150
Solid	-24.094008	5.389302	17.203406	-5.987984	.687804	.147513	6.210096
88	Be ₂ Cl ₄						
Gas	-199.512790	29.976862	1.196290	-.270883	.020314	-1.744455	93.079212
89	Be ₂ O ₂						
Gas	-110.915340	18.683342	.795030	-.184122	.014118	-.925398	77.771712
90	Be ₃ N ₂ -s,1						
Liquid	-116.447000	34.999996	.000005			-.000001	54.980300
Solid	-142.102940	22.067825	13.641458	-3.078478	-.003661	-.877109	29.847476
91	Be ₃ O ₃						
Gas	-274.948220	29.404571	1.570326	-.355216	.026616	-2.000817	89.410432

Constants for the Generation of Thermodynamic Properties (Contd.)

	17	11	12	13	14	15	16
92	Be ₂ O ₄						
Gas	-397.881920	40.530396	2.093584	-.473440	.035467	-2.694566	107.304050
93	Be ₂ O ₅						
Gas	-519.812840	51.653150	2.620631	-.593058	.044462	-3.387942	124.530420
94	Be ₂ O ₆						
Gas	-662.844080	62.773790	3.149658	-.712988	.053463	-4.081012	141.350760
95	C-s						
Solid	-3.236550	5.364067	.454333	-.093518	.008848	-.518240	5.193956
96	C						
Gas	169.321130	5.128910	-.256669	.124645	-.011837	-.014314	43.969762
97	CCl						
Gas	128.892930	8.831985	.104301	-.016420	.001234	-.147797	63.690944
98	CClFO						
Gas	-110.083420	18.211480	1.076220	-.241617	.018022	-.825362	83.794622
99	CClF ₃						
Gas	-176.074850	24.635770	.789295	-.178995	.013444	-1.164086	91.881968
100	CClN						
Gas	27.105596	12.993748	1.226510	-.270344	.020060	-.369982	59.961118
102	CCl ₃ F						
Gas	-75.162512	25.299489	.351537	-.079429	.005942	-.811036	100.328400

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
103	CCl ₄						
Gas	-35.665472	25.539650	.194668	-.044259	.003330	-.649833	101.477910
104	CF						
Gas	71.129452	8.472163	.390032	-.069075	.005152	-.235639	59.906204
105	CFN						
Gas	-8.274402	12.748741	1.371245	-.304816	.022606	-.451247	66.727922
106	CF ₂						
Gas	-51.754364	12.979625	.703464	-.138361	.010374	-.592516	70.016770
107	CF ₂ O						
Gas	-159.467480	17.807903	1.336454	-.299813	.022353	-.985744	78.125662
108	CF ₃						
Gas	-138.473010	18.500594	.898134	-.202963	.015210	-.926457	79.881582
109	CF ₄						
Gas	-229.517860	24.221224	1.059553	-.239855	.017990	-1.344073	84.758022
110	CH						
Gas	139.998010	6.324556	1.724714	-.347737	.025417	-.019289	50.825316
111	CHClF ₂						
Gas	-122.410320	21.214349	2.878290	-.631814	.046481	-1.262587	85.010592
112	CHCl ₂ F						
Gas	-71.004078	21.642003	2.600818	-.569803	.041885	-1.091300	90.020426
113	CHCl ₃						
Gas	-34.603932	21.996968	2.366056	-.516379	.037859	-.928909	91.921538
114	CHFO						
Gas	-97.595732	14.852859	3.137170	-.690039	.050837	-.975824	71.324160

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
115	CHF ₃						
Gas	-173.383280	20.828625	3.129198	-.688270	.050696	-1.418625	79.391084
116	HCN						
Gas	26.979230	9.986136	3.250734	-.651461	.047056	-1.353130	57.630370
117	CHNO						
Gas	-34.228678	14.074463	3.496895	-.753186	.054768	-.631866	69.814306
118	CHO						
Gas	-7.112880	9.606640	2.664107	-.582820	.042800	-.403585	62.660910
119	CH ₂						
Gas	62.118256	8.103459	4.147580	-.899150	.065644	-.423667	49.848576
120	CH ₂ ClF						
Gas	-67.546064	18.009842	4.832264	-1.055696	.077455	-1.274683	77.370188
121	CH ₂ Cl ₂						
Gas	-31.652748	18.513698	4.503238	-.981407	.071891	-1.131238	80.140592
122	CH ₂ F ₂						
Gas	-115.409340	17.547138	5.145811	-1.127498	.082862	-1.438133	71.740404
123	CH ₂ O						
Gas	-34.505852	12.186877	4.805755	-1.057404	.077920	-.968787	61.108172
124	CH ₃						
Gas	26.003928	11.262893	5.356246	-1.174951	.086414	-.765771	54.645838
125	CH ₃ Cl						
Gas	-29.120522	15.007863	6.654601	-1.449382	.106124	-1.204770	66.286470
126	CH ₃ Cl ₃ Si						
Gas	-135.288130	22.600720	21.427670	-9.356010	1.541070	-.389553	103.161430

Constants for the Generation of Thermodynamic Properties (Contd.)

	17	11	12	13	14	15	16
127	CH ₃ F						
Gas	-67.769140	14.474479	7.021297	-1.534494	.112604	-1.350646	62.361040
128	CH ₃ F ₃ Si						
Gas	-303.126620	19.301320	27.139140	-13.214180	2.491270	-.509665	88.204722
129	CH ₄						
Gas	-25.160290	11.661670	8.707460	-1.895976	.138799	-1.120690	50.904648
130	MgCO ₃ -s						
Solid	-274.237580	20.595900	8.073000	6.261000	-2.478000	-.506930	35.143878
131	CN						
Gas	88.510436	7.388968	.633676	.165751	.028860	-.147159	56.488444
132	NaCN-s, 1						
Liquid	-24.594028	20.999990	.000009	.000003		.000002	57.671964
Solid	-25.763984	13.000050	10.000100	-.000330	.000050	-.000002	42.643906
133	NaCN						
Gas	26.565990	12.999997	.000001			.000001	83.144004
134	NaCO ₃ -s						
Liquid	-284.473240	47.388440	.979640	-.375560	.048656	-1.512106	82.488524
Solid	-337.696440	140.162560	-180.285920	120.392550	-24.306690	-10.632385	199.996480
135	CO						
Gas	-29.109842	7.263554	1.103525	-.235811	.017634	-.159392	54.979636
136	COS						
Gas	-38.669236	13.154942	1.277352	-.249812	.018566	-.511373	68.338456
137	CO ₂						
Gas	-99.623754	12.226062	1.789351	-.380132	.029171	-.590839	62.475718

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
138 CP							
Gas	89.705870	8.542839	.314457	-.058855	.004402	-.236227	60.769028
139 CS							
Gas	68.206246	8.497865	.339804	-.065295	.004871	-.240513	59.329988
140 CS ₂							
Gas	22.298244	14.072677	.576108	-.121729	.009092	-.462859	71.388380
141 CS ₁ -s							
Solid	-17.705031	9.996904	1.786304	.019390	-.004791	-.368576	13.438009
142 CT ₁ -s,1							
Liquid	-30.742006	12.999997	.000001			.000001	24.182002
Solid	-48.579372	11.854710	.761283	.019606	-.003139	-.362467	17.906981
143 C ₂							
Gas	195.956190	6.792445	1.805289	-.355200	.023236	.314701	57.044328
144 C ₂ F ₂							
Gas	-59.057580	18.844614	1.298102	-.290115	.021591	-.662207	79.407850
145 C ₂ F ₄							
Gas	-165.024010	29.023056	1.803639	-.405821	.030311	-1.459301	99.849168
146 C ₂ H ₂							
Gas	48.649000	12.704947	5.180604	-1.038340	.075106	-.482764	59.438028
147 C ₂ H ₄							
Gas	2.124806	17.412427	8.809391	-1.914535	.139984	-1.547497	63.522214
148 C ₂ H ₄ O							
Gas	-26.119568	22.585753	9.333424	-2.034061	.149000	-2.184897	72.119502

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
149	$\text{Li}_2\text{C}_2\text{-s}$						
Solid	-24.005082	24.469500	2.204310	.136620	-.025576	-.720667	38.911014
150	$\text{MgC}_2\text{-s}$						
Solid	14.648259	17.017755	1.544050	-.000750	-.000355	-.359886	31.108470
151	C_2N_2						
Gas	66.657956	17.113022	2.381911	-.528647	.039168	-.640429	74.606248
152	C_3						
Gas	184.069830	12.648416	1.442686	-.321489	.023872	-.565843	62.829372
153	$\text{Mg}_2\text{C}_3\text{-s}$						
Solid	8.384323	28.440140	2.447890	.067780	-.013221	-.604847	54.289946
154	C_3O_2						
Gas	-18.472851	22.241892	2.925825	-.651268	.048335	-1.088006	81.967940
155	C_4						
Gas	234.443060	17.609287	2.082690	-.464036	.034450	-.810482	74.832162
156	$\text{C}_4\text{H}_{12}\text{Si-s}$						
Gas	-77.822886	15.438710	80.784800	-33.627600	5.108230	-.438265	80.040874
157	C_4N_2						
Gas	115.734160	27.050822	3.649160	-.810554	.060071	-1.129570	95.466932
158	C_5						
Gas	232.218640	22.570146	2.722714	-.606584	.045028	-1.055122	80.965504
159	Cl						
Gas	27.253020	5.613747	-.400034	.087661	-.006445	.000290	46.317924
160	ClF						
Gas	-16.858370	9.227216	-.305960	.158624	-.015773	-.194730	62.326988
161	Li_2ClF						
Gas	-187.751950	19.611524	.174089	-.039865	.003010	-.524496	84.962408

Constants for the Generation of Thermodynamic Properties (Contd.)

	17	11	12	13	14	15	16
162	MgClF						
Gas	-144.231910	14.833033	.048156	-.011131	.000851	-.276860	76.087262
163	FC10 ₃						
Gas	-16.303092	24.454744	.906356	-.205192	.015390	-1.214639	89.864412
164	ClF ₃						
Gas	-46.241098	19.704880	.111571	-.025393	.001908	-.458640	89.414902
165	SiClF ₃						
Gas	-325.062320	25.384624	.297081	-.067448	.005066	-.771485	100.383770
166	HCl						
Gas	-23.844752	6.169057	1.765351	-.361643	.026302	.009848	51.680660
167	HOCl						
Gas	-25.889486	10.092730	2.218470	-.466771	.033430	-.249864	66.866336
168	SiClH ₃						
Gas	-58.344798	19.992095	3.724137	-.828455	.061457	-1.349683	76.421038
169	NH ₄ Cl						
Solid	-111.439760	69.180130	-59.364580	32.632400	-6.178204	-6.220941	96.310762
170	NH ₄ ClO ₄						
Solid	-91.810294	70.699200	.005000	.003000	-.001000	-.000040	126.053420
171	LiCl-s,1						
Liquid	-97.666966	14.400003	-.000009	-.000001	-.000001	-.000001	33.526212
Solid	-100.931150	10.616830	4.695360	.037440	-.023284	-.048498	23.512954
172	LiCl						
Gas	-46.830008	8.896482	.163814	-.007491	.000576	-.114148	60.951110

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
173	LiOCl						
Gas	-8.807584	13.517402	.258785	-.058547	.004384	-.429426	75.369930
174	LiClO ₄ -s,1						
Liquid	-98.730764	32.819880	19.999900		-.000020	-.000019	68.886424
Solid	-100.771170	29.022300	27.483000	-.018000	.010000	-.002560	56.617998
175	MgCl						
Gas	-1.879457	8.927568	.125591	-.002714	.000215	-.064429	66.139730
176	NOCl						
Gas	7.658387	12.698095	1.149883	-.176049	.013119	-.360167	75.808460
177	NaCl-s,1						
Liquid	-97.989990	16.000006	.000002	-.000004			39.582498
Solid	-101.682250	10.979990	3.899990	-.000010	-.000009	-.000001	29.437456
178	NaCl						
Gas	-46.863648	8.937650	.181807	-.000970	.000086	-.042580	65.407250
179	ClO						
Gas	21.013860	8.815760	.194330	-.019091	.001431	-.169833	63.890566
180	ClO ₂						
Gas	19.467665	13.422319	.495070	-.072557	.005437	-.477099	75.159688
181	SiCl						
Gas	45.287602	8.931160	.099835	-.001465	.000101	-.044681	67.241234
182	TiCl						
Gas	14.119456	8.933987	.196907	-.000992	.000064	-.063300	69.221068
183	Cl ₂						
Gas	-3.230782	9.366107	-.439384	.213974	-.021676	-.143300	64.013784

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
184	SiH ₂ Cl ₂						
Gas	-85.086738	21.900065	2.509708	-.558630	.041460	-.1.092863	88.845210
185	Id ₂ Cl ₂						
Gas	-147.930820	19.772043	.065829	-.014743	.001092	-.376854	89.530432
186	MgCl ₂ -s,1						
Liquid	-151.568010	22.100008	-.000016	.000008		.000001	54.758430
Solid	-159.748630	19.244470	.689390	.500160	-.109636	-.227634	43.279108
187	MgCl ₂						
Gas	-105.745610	14.864795	.026150	-.005921	.000444	-.186362	78.467794
188	Cl ₂ O						
Gas	12.889794	13.667817	.150710	-.036491	.002741	-.352598	78.336520
189	SiCl ₂						
Gas	-42.383474	13.872430	.023724	-.004982	.000344	-.179023	82.853848
190	TiCl ₂ -s,1						
Liquid	-124.948920	21.000003	-.000020	-.000002			52.103068
Solid	-128.120350	16.599980	3.000010	-.000020	-.000005	-.000001	42.687330
191	TiCl ₂						
Gas	-77.698016	13.999996	.000003				76.012244
192	ZrCl ₂ -s,1						
Liquid	-147.543990	23.000007	.000014	-.000007	-.000004	-.000003	57.281598
Solid	-150.317900	17.299960	4.200000	-.000020	-.000019	-.000001	46.760344
193	ZrCl ₂						
Gas	-96.333818	13.907852	.001115	-.000026	-.000014	-.056351	84.843278
194	SiCl ₃ F						
Gas	-210.131140	25.636362	.130848	-.029572	.002207	-.455918	108.868700

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
195	SiHCl ₃						
Gas	-121.573570	23.698517	1.359496	-.302122	.022392	-.766885	99.269572
196	I ₂ Cl ₃						
Gas	-240.264560	31.526010	.179545	-.040961	.003092	-.785982	114.150210
197	POCl ₃						
Gas	-144.165550	25.293918	.354533	-.080113	.005996	-.625478	104.612360
198	PCl ₃						
Gas	-69.275700	19.825066	.030886	-.006890	.000512	-.262213	97.126332
199	PSCl ₃						
Gas	-100.135510	25.701542	.088422	-.020260	.001537	-.449471	109.196860
200	TiCl ₃ -s						
Solid	-180.089850	24.274450	1.874650	1.226700	-.236886	297210	60.616036
201	TiCl ₃						
Gas	-138.004080	19.071326	.199797	-.005033	.000434	-.165006	96.979876
202	ZrCl ₃ -s,1						
Liquid	-209.882980	31.500006	-.000002	-.000001			79.172676
Solid	-214.957760	21.399980	12.999930	-.000130	-.000020	-.000001	56.521636
203	ZrCl ₃						
Gas	-160.216070	19.860821	.007328	-.001627	.000124	-.149026	105.716900
204	SiCl ₄						
Gas	-154.775230	25.720683	.075622	-.017281	.001307	-.428836	108.067540
205	TiCl ₄						
Gas	-191.06630	25.784611	.031029	-.006583	.000462	-.296885	113.788330

Constants for the Generation of Thermodynamic Properties (Contd.)

	17	13	12	13	14	15	16
206	ZrCl ₄ -s,1						
Liquid	-241.517040	40.000020	-.000010	.000010		-.000003	97.224636
Solid	-244.593960	31.913700	.009020	-.004052	.000562	-.290319	81.484200
207	ZrCl ₄						
Gas	-216.073080	25.802179	.021222	-.004771	.000357	-.232411	117.655970
208	PCl ₅						
Gas	-95.914434	31.686962	.072341	-.016485	.001245	-.557542	118.282210
209	F						
Gas	17.539261	5.070510	-.066876	.015150	-.001136	.060321	44.365718
210	HF						
Gas	-65.661692	5.385666	2.006661	-.385756	.026779	.169273	48.254026
211	HO ₂						
Gas	-30.029304	9.880022	2.356958	-.498094	.035785	-.283613	63.919390
212	SiH ₃ F						
Gas	-115.678170	19.827898	3.831330	-.852566	.063251	-1.471835	72.756042
213	LiF-s,1						
Liquid	-145.285970	15.310006	-.000006	-.000002		-.000001	28.811490
Solid	-144.507140	1.793866	19.137859	-8.605517	1.252471	.615758	8.215178
214	LiF						
Gas	-82.502574	8.794453	.234800	-.022511	.001696	-.179610	57.483638
215	LiOF						
Gas	-15.564964	13.420635	.321702	-.072686	.005439	-.488749	72.546926
216	MgF						
Gas	-24.082146	8.881695	.132800	-.009070	.000681	-.132728	62.871228

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
217 NF							
Gas	55.364266	8.750545	.127583	-.029119	.002200	-.196583	58.458050
218 FNO							
Gas	-20.878960	12.617978	.835367	-.187304	.013961	-.440396	72.144164
219 NaF-s,1							
Liquid	-136.143960	16.400009	-.000013	-.000001			33.246772
Solid	-139.736280	10.531951	3.581420	.208253	-.034607	-.040103	23.700488
220 NaF							
Gas	-69.971412	8.912101	.116940	-.005034	.000393	-.094841	61.943768
221 OF							
Gas	29.164712	8.749673	.128706	-.029563	.002253	-.196479	60.299150
222 PF							
Gas	-20.220900	8.779595	.178038	-.024213	.001820	-.187947	63.347868
223 PSF							
Gas	-46.290746	13.665276	.162989	-.037224	.002812	-.377454	80.896422
224 SiF							
Gas	7.204554	8.828964	.152530	-.016764	.001256	-.144049	63.865276
225 F2							
Gas	-3.215851	8.791140	.307074	-.022521	.001695	-.183065	58.069530
226 SiH2F2							
Gas	-205.091220	21.203976	2.966383	-.661769	.049177	-1.482719	79.834293
227 Li2F2							
Gas	-221.400500	19.520489	.232408	-.052659	.003945	-.642756	81.509030

Constants for the Generation of Thermodynamic Properties (contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
228	MgF ₂ -s,1						
Liquid	-260.151000	22.570001	.000008	-.000001		.000001	42.687156
Solid	-268.551180	16.997741	2.445019	.023267	-.001731	-.228963	32.199366
229	MgF ₂						
Gas	-182.557060	14.767466	.091712	-.021131	.001610	-.354062	71.858886
230	F ₂ O						
Gas	2.206879	13.634567	.181763	-.041176	.003088	-.412886	73.475292
231	SiOF ₂						
Gas	-121.039570	19.158875	.470548	-.106893	.008042	-.723609	85.942742
232	SiO ₂ F ₂						
Gas	-160.972990	24.367317	.961483	-.217340	.016282	-1.156690	91.757116
233	PF ₂						
Gas	-114.272180	13.680987	.153426	-.035236	.002677	-.370057	76.810306
234	SiF ₂						
Gas	-123.493740	13.463370	.293605	-.066350	.004968	-.463302	74.612542
235	TiF ₂ -s,1						
Liquid	-217.344960	21.000001	.000003	-.000004		-.000001	45.293066
Solid	-222.398000	13.700010	7.000000	.000003	-.000003	-.000002	32.484894
236	TiF ₂						
Gas	-137.392540	13.582158	.217939	-.049644	.003739	-.418547	79.459434
237	ZrF ₂ -s,1						
Liquid	-229.324940	29.999994	-.000002	-.000001			59.809414
Solid	-236.281920	19.399950	11.200000	.000010	-.000010	-.000002	41.138682

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
238	ZrF ₂						
Gas	-151.709700	13.805820	.069629	-.015864	.001195	-.274455	76.564646
239	SiHF ₃						
Gas	-293.624140	23.024656	1.798295	-.400895	.029775	-1.166076	87.847966
240	Id ₃ F ₃						
Gas	-370.856320	30.934584	.566633	-.128061	.009579	-1.253769	101.958210
241	NF ₃						
Gas	-38.116320	19.281557	.389141	-.088142	.006613	-.829480	81.254630
242	PF ₃						
Gas	-228.649720	19.467715	.268232	-.061011	.004591	-.664787	85.199578
243	TiF ₃ -s,1						
Liquid	-332.425940	28.000013	-.000019	-.000002	-.000004	-.000001	59.894000
Solid	-340.827040	17.200030	11.200010	.000010		-.000001	39.473978
244	TiF ₃						
Gas	-263.131520	19.586070	.189882	-.043217	.003254	-.613904	88.723248
245	ZrF ₃ -s,1						
Liquid	-347.424880	31.999986	-.000002	-.000004		.000002	69.872858
Solid	-357.096860	22.400006	9.399970	-.000006		-.000001	51.303888
246	ZrF ₃						
Gas	-278.295380	19.755502	.076867	-.017315	.001292	-.398942	92.054550
247	SiF ₄						
Gas	-383.472280	25.041120	.523246	-.118631	.008902	-.967048	92.657644
248	TiF ₄ -s						
Solid	-398.869340	15.399900	40.003800	-.003700	.000800	.000070	38.728878

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
249	TiF ₄						
Gas	-379.388060	25.486691	.229323	-.051973	.003897	-.676461	101.604580
250	ZrF ₄ -s,1						
Liquid	-447.898100	18.098098	23.820150	-10.815635	1.583001	.369465	53.548232
Solid	-470.102400	33.278999	.121270	-.095903	-.002194	-1.083846	59.782562
251	ZrF ₄						
Gas	-408.547500	25.644064	.127194	-.029240	.002225	-.521908	105.168300
252	SF ₆						
Gas	-304.713320	36.929326	.546311	-.123944	.009294	-1.605729	105.867520
253	H						
Gas	50.621310	4.967999	.000002				33.404545
254	LiH						
Gas	28.814984	8.375470	.579567	-.082492	.006138	-.247350	49.619288
255	LiOH-s,1						
Liquid	-120.235960	20.740000	-.000010	-.000002	.000001	-.000001	36.633790
Solid	-116.818910	1.264480	31.574950	-16.308700	2.800367	.469782	5.229932
256	LiOH						
Gas	-61.685642	9.744508	2.399972	-.502415	.035875	-.315344	62.165864
257	MgH						
Gas	37.440840	8.300312	.526014	-.095072	.007133	-.247611	54.867620
258	MgOH						
Gas	-16.072417	10.062525	2.244506	-.473492	.033976	-.247413	68.047888

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
259 NH							
Gas	77.566954	5.871481	1.935644	-.387239	.027959	.062003	50.161504
260 NaH							
Gas	26.579168	8.613321	.445306	-.048135	.003587	-.228348	54.179236
261 NaOH-s,1							
Liquid	-105.062170	19.083680	.840108	-.266859	.028207	.324866	41.996290
Solid	-121.630220	43.420390	-36.858360	21.190120	-4.145827	-2.950127	65.767932
262 NaOH							
Gas	-59.081066	10.088060	2.212412	-.464186	.033176	-.172592	67.620396
263 OH							
Gas	8.059381	5.539488	2.029926	-.402411	.028569	.147895	50.760544
264 PH							
Gas	52.385620	6.986268	1.355447	-.271294	.020027	-.124918	54.421950
265 HS							
Gas	32.826868	6.534243	1.598349	-.324816	.023830	-.054298	54.536912
266 SiH							
Gas	111.162000	7.455745	1.110821	-.211426	.015711	-.187816	55.279614
267 H ₂							
Gas	-1.059953	5.290330	2.024190	-.352047	.024860	.193870	37.936122
268 I4O2H ₂							
Gas	-181.136920	22.944479	5.142059	-1.082201	.077536	-1.479660	78.737222
269 MgH ₂ -s							
Solid	-25.955370	18.420552	-10.860800	7.613660	-1.766407	-.929447	28.149334

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
270	MgO ₂ H ₂ -s						
Solid	-227.729360	18.469400	9.650000	5.625000	-1.764700	-.185570	32.937540
271	NH ₂						
Gas	37.989890	6.726628	4.233935	-.898776	.064741	-.047498	51.859186
272	H ₂ O						
Gas	-59.597646	6.083043	4.622610	-.933442	.066088	.061312	51.465054
273	H ₂ O ₂						
Gas	-37.707634	12.720020	2.893730	-.090740	-.104430	-.392794	68.163596
274	H ₂ SO ₄ -l						
Liquid	-201.987400	24.230540	37.989140	-24.396200	5.114660	.233648	57.407636
275	PH ₂						
Gas	55.032030	9.835376	2.576715	-.570582	.042213	-.450341	59.875316
276	SiH ₂						
Gas	-8.507971	8.625942	3.434304	-.716336	.052611	-.320397	57.138274
277	NH ₃						
Gas	-14.645140	7.831464	7.080605	-1.501533	.108113	-.323726	51.928286
278	H ₃ PO ₄ -s,1						
Liquid	-313.661120	48.000070	.000050	.000030	-.000020	-.000006	96.387798
Solid	-343.298120	114.656700	-231.981200	267.058400	-104.969500	-4.765040	198.603180
279	PH ₃						
Gas	-.813127	13.276554	4.181543	-.927203	.068639	-1.007777	60.333502
280	N ₂ H ₄						
Gas	16.611584	14.543000	7.096630	3.062790	-1.892760	-.430086	69.863322

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
281	SiH ₄						
Gas	-2.632605	18.153918	4.897658	-1.089702	.080843	-1.550359	61.926646
282	Li-s,l						
Liquid	-1.314616	7.080335	-.382112	.140542	-.016171	.069401	17.120514
Solid	-2.508972	7.615038	-.569250	.327251	-.064031	-.045563	15.763572
283	Li						
Gas	36.834498	5.103289	-.104315	-.026272	.024037	-.019892	39.259726
284	LiN						
Gas	35.809592	8.175167	.577669	-.113739	.008488	-.239407	59.326202
285	LiO						
Gas	10.723379	8.400532	.427013	-.080422	.006031	-.244172	58.890424
286	Li ₂						
Gas	47.590724	8.934596	.329650	-.001462	.000114	-.039268	57.548064
287	Li ₂ O-s,l						
Liquid	-139.174930	23.000002	-.000006	-.000004			37.694352
Solid	-148.440750	14.899548	6.160570	-.056622	.013316	-.335083	23.286554
288	Li ₂ O						
Gas	-39.796262	13.396744	.336936	-.075968	.005672	-.533482	69.464822
289	Li ₃ N-s						
Solid	-55.316516	17.993510	22.945670	-15.237300	3.254832	-.458482	21.952540
290	Mg-s,l						
Liquid	.419915	5.277602	2.619245	-.007666	.000917	-.010106	15.684376
Solid	-.477917	2.770681	6.585290	-1.723270	.345766	.202559	10.270231

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
291	Mg						
Gas	33.877512	4.892170	.179632	-.136045	.030886	.004041	41.397328
292	MgO-s						
Solid	-148.140390	11.347224	1.716498	-.592647	.073251	-.303114	18.068232
293	MgO						
Gas	1.062427	8.853366	.157550	-.013162	.000976	-.149994	60.839506
294	MgSiO ₃ -s,1						
Liquid	-371.493360	33.808238	3.115617	-.963576	.100105	-2.888419	47.614966
Solid	-373.301040	26.130450	2.400660	1.177697	-.191592	-.797808	42.723856
295	MgSO ₄ -s,1						
Liquid	-326.346760	30.707960	25.186680	-9.960330	1.341266	-4.313216	35.813154
Solid	-311.168600	15.891410	23.264440	-1.042340	.230260	.027015	34.396660
296	MgS-s						
Solid	-85.873318	9.250017	2.500014	-.000009	-.000001	-.000001	21.436704
297	MgS						
Gas	30.278596	8.925893	.010396	-.002190	.000154	-.079891	67.762430
298	Mg ₂ SiO ₄ -s,1						
Liquid	-523.605200	48.133940	3.986890	-1.237206	.126904	-3.927548	67.543900
Solid	-527.086320	36.356300	5.676470	.381230	-.037642	-.903778	59.993932
299	Mg ₂ Si-s,1						
Liquid	-7.500006	22.500008	-.000005	.000001			56.789540
Solid	-24.610466	17.418627	3.572550	.209790	-.115220	-.133236	38.392312
300	Mg ₃ N ₂ -s						
Solid	-120.373970	27.630730	4.580040	-2.838140	.531852	-.704426	50.367150

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
301	Mg ₃ P ₂ O ₈ -s,1						
Liquid	-933.258320	92.371880	4.472330	-1.404660	.147706	-6.006343	126.407850
Solid	-911.157640	45.330990	38.461980	2.060570	-.304130	-.584794	85.125750
302	N						
Gas	111.392770	5.104901	-.136980	.022207	.004887	-.018643	42.745226
303	NO						
Gas	18.744525	7.674605	.862283	-.182096	.013546	-.193729	58.524526
304	NO ₂						
Gas	2.359917	12.486581	.927845	-.208851	.015597	-.623810	69.166918
305	PN						
Gas	18.308411	8.436739	.377472	-.074813	.005604	-.242868	59.380122
306	NS						
Gas	59.851228	8.567751	.308864	-.056203	.004228	-.189166	62.444114
307	SiN						
Gas	117.712610	8.623190	.269171	-.047745	.003589	-.225573	61.049006
308	TiN-s,1						
Liquid	-69.266994	13.499997	.000002	-.000001			25.826828
Solid	-85.086192	11.904955	.937349	.005190	-.001300	-.296190	19.659744
309	ZrN-s,1						
Liquid	-73.462376	11.127090	2.321936	-.584313	.046595	-.223952	26.593178
Solid	-91.263454	11.102334	1.677631	.000619	-.000049	-.172326	21.251010
310	N ₂						
Gas	-2.486823	6.973146	1.274237	-.274263	.020277	-.118559	53.318418

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>13</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
311 N ₂ O							
Gas	13.859506	12.615769	1.462495	-.325805	.024137	-.580897	64.571162
312 N ₂ O ₃							
Gas	9.886999	23.191949	1.713949	-.384981	.028722	-1.058318	96.363930
313 N ₂ O ₄							
Gas	-11.238626	28.519676	2.129959	-.479038	.035767	-1.567590	98.829954
314 N ₂ O ₅							
Gas	-13.515669	34.026953	2.429875	-.547112	.040884	-2.012556	106.216730
315 Si ₃ N ₄ -s							
Solid	-179.842690	4.311000	49.454320	-16.292290	1.772628	.860841	18.286594
316 P ₃ N ₅ -s							
Solid	-78.645180	12.270630	61.678170	-28.015910	4.101363	.913413	46.613850
317 Na-s, l							
Liquid	-2.815188	11.280620	-10.314610	7.643958	-1.562591	-.134248	29.556202
Solid	-2.464839	7.999940	.000100	-.001100	.000210	.000002	21.739644
318 Na							
Gas	24.980838	3.778435	1.631630	-.728519	.107934	.135597	41.472904
319 NaO							
Gas	10.158282	8.893911	.160650	-.007379	.000555	-.118115	64.151816
320 Na ₂							
Gas	30.155478	8.946818	.380721	.001285	-.000116	-.009121	65.657172

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
321	Na ₂ O-s,1						
Liquid	-100.379550	23.999993	-.000011	.000002			48.173674
Solid	-104.320940	15.699980	5.400000	-.000010	-.000014		34.789694
322	Na ₂ SiO ₃ -s,1						
Liquid	-369.413760	43.115911	.852509	-.257077	.026179	-2.022543	75.737758
Solid	-373.132140	31.862120	7.855460	1.511900	-.444850	-.690584	59.608388
323	Na ₂ Si ₂ O ₇ -s,1						
Liquid	-596.710080	62.450930	4.449330	-1.365656	.141253	-4.869901	100.672420
Solid	-590.015580	44.520390	16.608960	.073310	.045920	-1.077288	82.447956
324	Na ₂ S-s,1						
Liquid	-95.772686	21.913349	.169723	-.070770	.009960	-.410187	48.339782
Solid	-94.529958	18.099970	3.000030	-.000020	-.000009		44.409316
325	O						
Gas	58.081640	5.107522	-.162870	.052985	-.003288	.010519	44.764060
326	P0						
Gas	-4.606800	8.557584	.303882	-.056797	.004241	-.191215	62.588712
327	S0						
Gas	-2.768323	8.625213	.265956	-.047287	.003543	-.225203	62.283064
328	Si0						
Gas	-24.704882	8.539369	.311713	-.059681	.004472	-.236467	59.650063
329	Ti0-s,1						
Liquid	-113.004990	14.499996	.000002	-.000001			31.497276
Solid	-133.763530	25.042523	-25.058750	18.219230	-3.514422	-1.202172	39.610356

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
330 TiO							
Gas	11.894128	8.735039	.189703	-.030331	.002319	-.188863	65.384190
331 ZrO							
Gas	20.434436	7.430978	-.289685	.062973	-.004609	.125174	66.622682
332 O ₂							
Gas	-3.082757	8.021190	.546042	.007775	-.006116	-.216097	57.546610
333 PO ₂							
Gas	-78.565842	13.469032	.290861	-.065873	.004937	-.484503	74.378786
334 SO ₂							
Gas	-76.585312	13.005321	.740367	-.133370	.009961	-.552852	72.120604
335 SiO ₂ -s,1							
Liquid	-210.675940	3.267316	20.334552	-7.141115	.301620	.137622	10.256798
Solid	-227.020940	33.533141	-23.097580	11.313710	-1.739858	-2.588822	4.526772
336 SiO ₂							
Gas	-79.783118	14.295497	.400278	-.090648	.006802	-.50606	69.262398
337 TiO ₂ -s							
Solid	-222.514840	12.141150	13.350710	-10.196670	2.747208	-.055201	22.514830
338 TiO ₂ -s,1							
Liquid	-217.984940	19.000000	-.000001	-.000004			38.422816
Solid	-231.977200	17.267437	1.126480	-.258062	.053745	-.378218	30.420044
339 TiO ₂							
Gas	-85.578202	14.471330	.284918	-.064614	.004855	-.457312	71.560022
340 ZrO ₂ -s,1							
Liquid	-251.480960	20.000000	-.000002			-.000001	37.634934
Solid	-271.129840	22.398697	-3.409967	.823937	-.064233	-1.173919	34.735200

Constants for the Generation of Thermodynamic Properties (Contd.)

	17	11	12	13	14	15	16
341	ZrO ₂						
Gas	-77.197966	14.574864	.217000	-.049198	.003691	-.421632	73.860208
342	O ₃						
Gas	29.047072	11.965927	2.317604	-.984604	.134746	-.408850	68.810710
343	SO ₃						
Gas	-103.477870	18.914115	1.809698	.193342	-.032500	-1.048307	78.506994
344	Ti ₂ O ₃ -s,1						
Liquid	-345.393940	35.999998	-.000001	-.000001		.000001	69.535290
Solid	-377.713060	36.209206	.131570	-.064203	.024098	-1.290489	56.080056
345	Ti ₃ O ₅ -s						
Solid	-597.877940	41.600030	8.000050	-.000070	-.000003	-.000002	84.596724
346	P ₄ O ₆ -s						
Gas	-704.714580	51.083486	.382528	-.085641	.006318	-1.407032	199.582530
347	P ₄ O ₁₀ -s						
Solid	-711.395020	5.331700	167.985000	-34.561000	4.317000	.114540	14.453590
348	P ₄ O ₁₀						
Gas	-718.187420	75.030190	2.929403	-.662932	.049702	-4.338345	160.432750
349	P-s						
Solid	-1.205590	3.837551	3.855380	-.261800	.051223	.036449	9.117028
350	P-s,1						
Liquid	2.446148	6.292003	.000001	.000002			17.863191
Solid	2.225986	6.329999	.000010	.000020	.000002	-.000001	17.312257
351	P						
Gas	77.64934	6.151183	-1.615799	.663240	-.061156	-.133362	46.243356

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
352 PS							
Gas	19.647062	8.911469	.088725	-.004433	.000317	-.059191	66.481164
353 P ₂							
Gas	39.556392	8.854769	.111965	-.013421	.001019	-.149131	62.022414
354 P ₄							
Gas	23.605790	19.793835	.051772	-.011682	.000872	-.383980	88.755234
355 P ₄ S ₃ -s,1							
Liquid	-49.196066	44.000020	.000020	.000010	-.000005	-.000003	102.757040
Solid	-47.434844	34.999990	-.000050	-.000090	-.000008	-.000002	90.355632
356 P ₄ S ₃							
Gas	-30.440002	36.999991	.000003				121.055720
357 Si-s,1							
Liquid	4.063520	-1.798016	14.971106	-8.476035	1.640271	1.326856	7.719378
Solid	-1.218192	3.376136	6.884510	-.018890	.004226	.001183	9.915331
358 Si							
Gas	65.418300	5.139423	-.221513	.121633	-.012464	.094618	46.819498
359 SiS							
Gas	13.823864	8.866381	.106888	-.011907	.000916	-.141241	63.392720
360 S ₂							
Gas	27.752548	8.880099	.103814	-.003973	.000564	-.135211	64.521638
361 SiS ₂ -s,1							
Liquid	-38.730586	3.801890	22.291630	-5.935470	-.087052	.211745	20.787330
Solid	-47.159994	12.899940	7.000070		.000016	.000004	29.516370

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
362 Sa							
Gas	9.528309	43.621657	.065053	-.014739	.001101	-.598157	152.782940
363 $Si-s,1$							
Liquid	10.266006	6.129998	.000001				18.628743
Solid	-2.061463	5.613075	1.037119	-.328726	.035551	-.105974	10.348968
364 Si							
Gas	109.125190	4.221513	.754595	-.144322	.009019	.132785	45.664910
365 Si_2							
Gas	131.116120	12.439821	-1.510325	.274051	-.016484	-.722278	67.031026
366 Si_3							
Gas	140.814240	14.858244	.031350	-.007227	.000546	-.199297	77.530560
367 $Ti-s,1$							
Liquid	1.493003	7.999998	.000002	-.000001			18.167172
Solid	-1.451618	5.925830	2.060649	-.562132	.096616	-.051922	14.128570
368 Ti							
Gas	111.780990	4.467361	-.080391	.497023	-.054038	.199833	49.463762
369 $Zr-s,1$							
Liquid	.476881	9.542918	-.709689	.163751	-.012419	-.584115	20.841346
Solid	-2.130086	7.389096	.190688	.171876	-.019570	-.158490	17.882283
370 Zr							
Gas	145.200860	4.408072	1.422026	-.105337	.001491	.375265	49.912876
371 $LaBO_2-s,1$							
Gas	-276.863280	54.825120	-18.435751	5.811510	-.610452	-7.032459	55.020628

Constants for the Generation of Thermodynamic Properties (Contd.)

	<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
373	CCl ₂ F ₂						
Gas	-10.740963	24.985195	.559021	-.126692	.009509	-.989307	96.945708
374	TlF						
Gas	-59.101938	8.869543	.126917	-.010974	.000820	-.140340	65.880238
375	LiNaO						
Gas	-71.421216	13.557494	.233400	-.053092	.003998	-.540605	75.425440
376	Li ₂ TiO ₃ -s,1						
Gas	-336.446600	-23.870384	98.040270	-43.809380	6.353690	4.359097	8.020211
378	MgTi ₂ O ₃ -s,1						
Gas	-565.140260	-13.936244	82.819040	-.28.231695	3.109851	5.383975	25.628946
379	Mg ₂ TiO ₄ -s,1						
Gas	-479.536400	-27.327780	93.405550	-32.280402	3.592968	6.430622	3.332577
380	N ₂ O ₄ -s,1						
Gas	-8.591929	22.716320	46.074100	-23.057100	.015060	.002010	64.717342

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